



UNIVERSITY  
*of York*

# Development and application of BOUT++ for large scale turbulence simulation

J. Leddy, B.Dudson, P.Hill, B.Shanahan, N.Walkden

PPPL Theory seminar  
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**EPSRC**  
Engineering and Physical Sciences  
Research Council

 **EUROfusion**

# Outline

## Numerical developments

- New coordinate system

- Flux-coordinate independent method

## A new plasma model (Hermes)

- 2-fluid cold ion model in divergence form

- Including neutral interactions

## Turbulence and Neutral Simulations

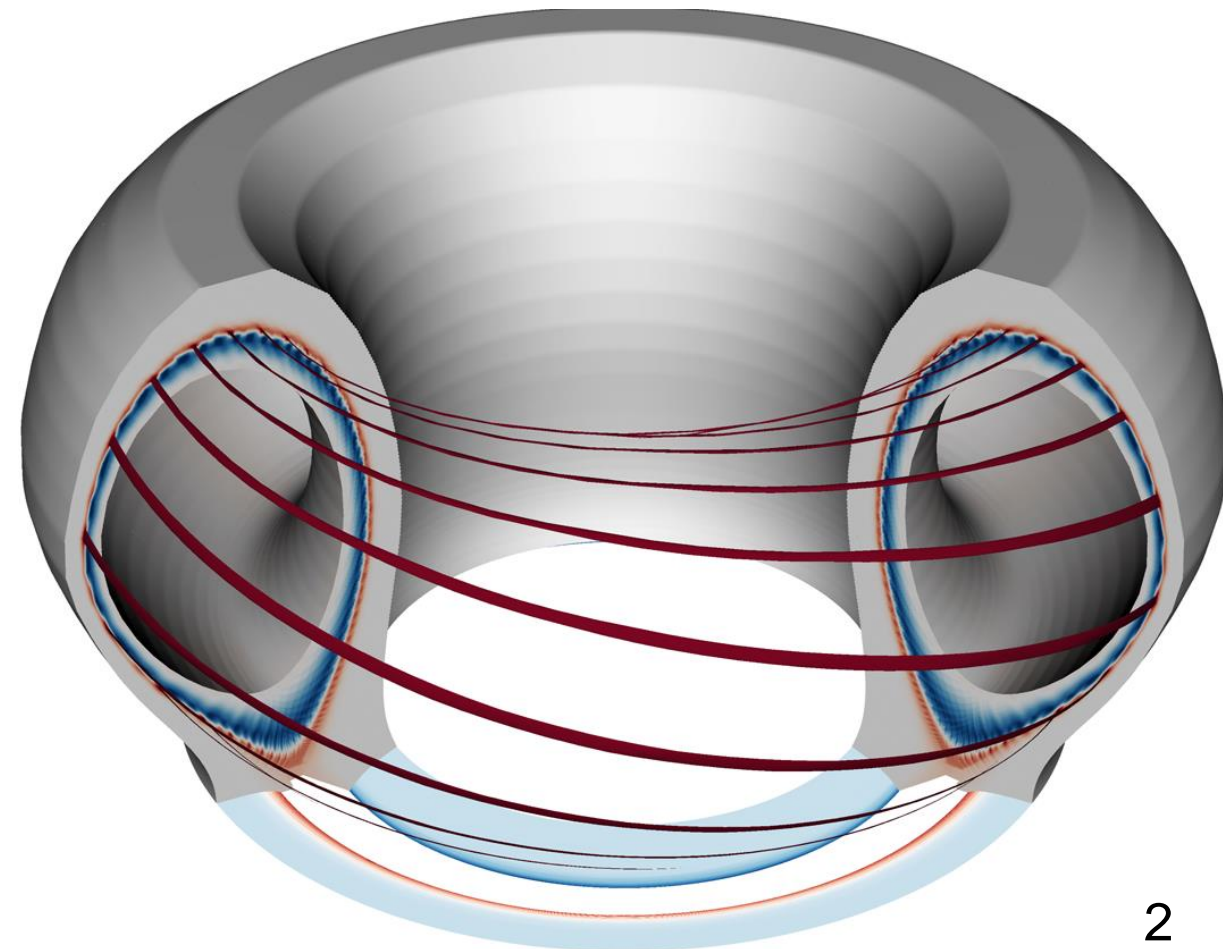
- Linear device

- MAST-U

- DIII-D

# What is BOUT++

- Framework for solving systems of PDE's
- Flexible numerical methods and geometries
  - Pvode, PETSc, grids from EFIT
- Easy to implement physics models
  - $\text{ddt}(\text{Ni}) = -\text{Div}(\text{Ni} * \text{Vi})$
- Designed with tokamaks in mind
  - Axisymmetry
  - Parallelization
- Open source at:  
<https://github.com/boutproject/BOUT-dev>



# Standard field-aligned coordinates

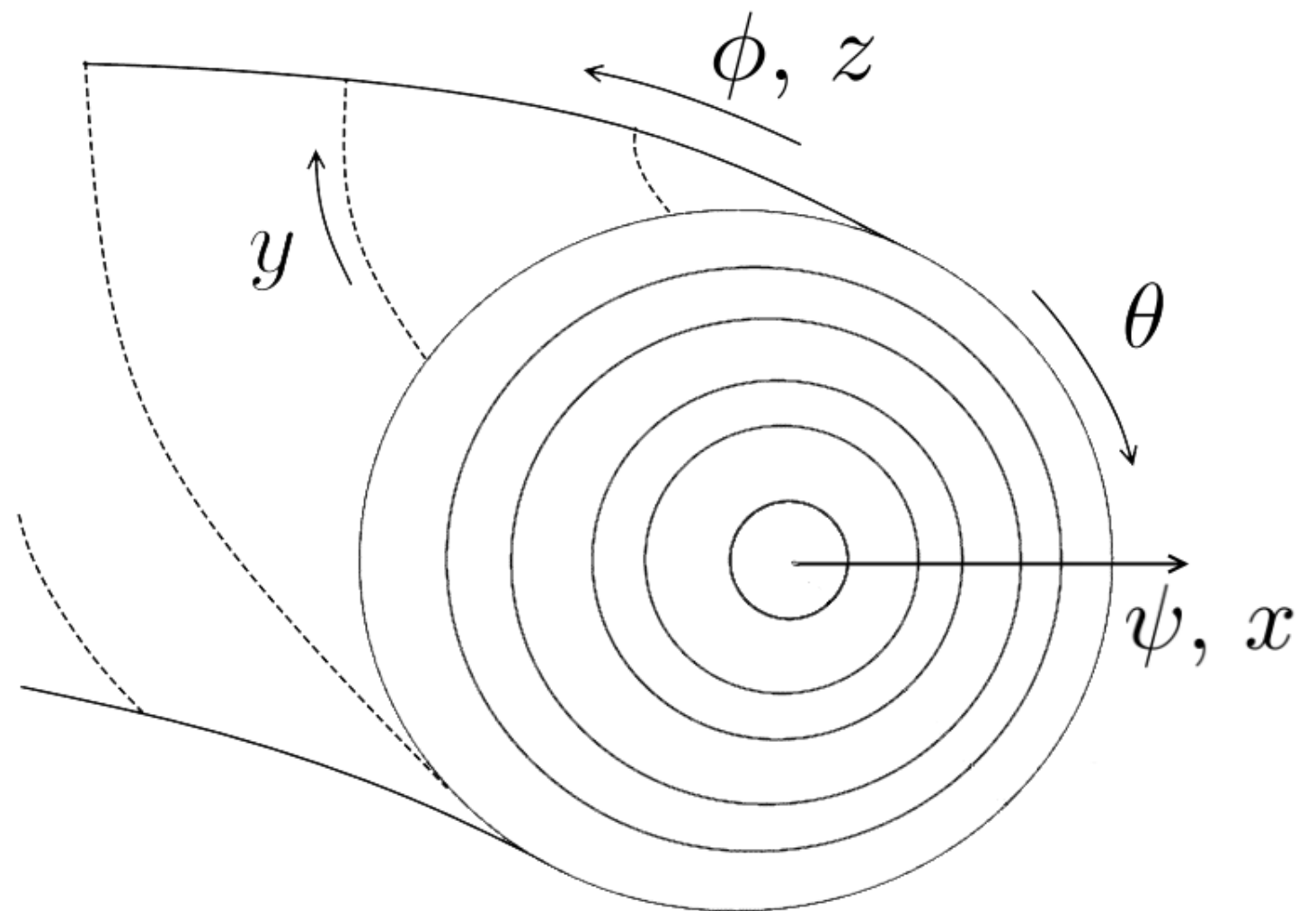
- Coordinate system should be **field-aligned**:
- Ease of parallel operations
- Perturbations tend to have low  $k_{\parallel}$

Coordinates:

$$x = \psi$$

$$y = \theta$$

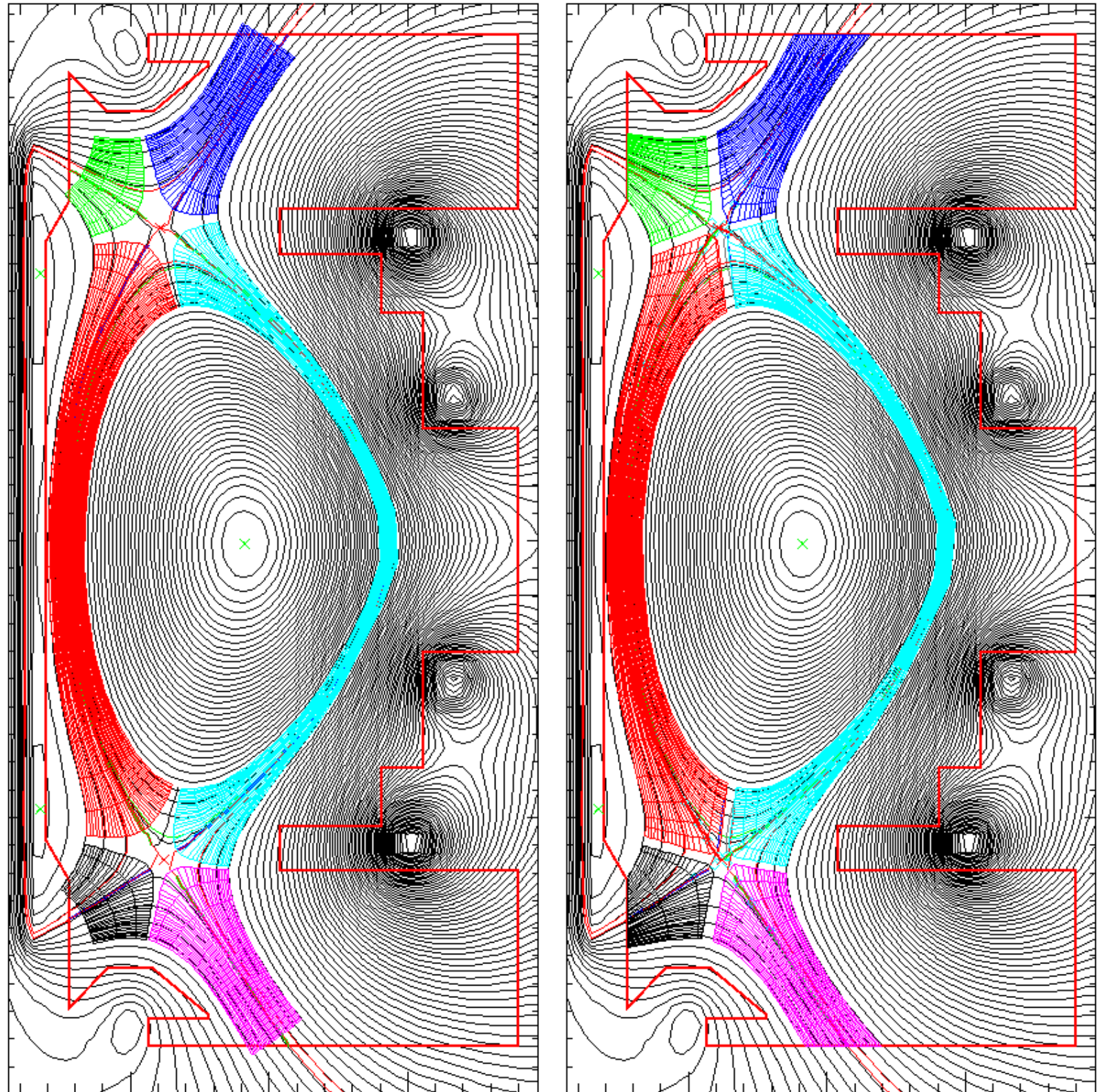
$$z = \phi - \int_{\theta_0}^{\theta} \nu \, d\theta$$





# Why new coordinates?

- Still desire field-aligned system
- But poloidal projection of  $x$  and  $y$  are constrained to be orthogonal
- With new coordinate system we can:
  - Match divertor geometry
  - Approach X-point more closely and evenly

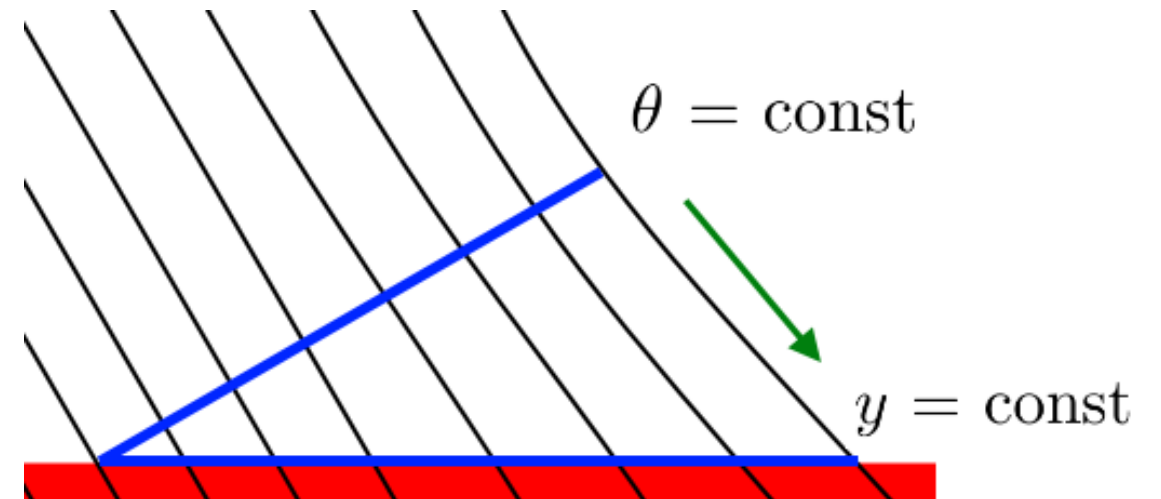


# Flexible field-aligned coordinates

$$x = \psi$$

$$y = \theta - \int_{\psi_0}^{\psi} \eta \, d\psi$$

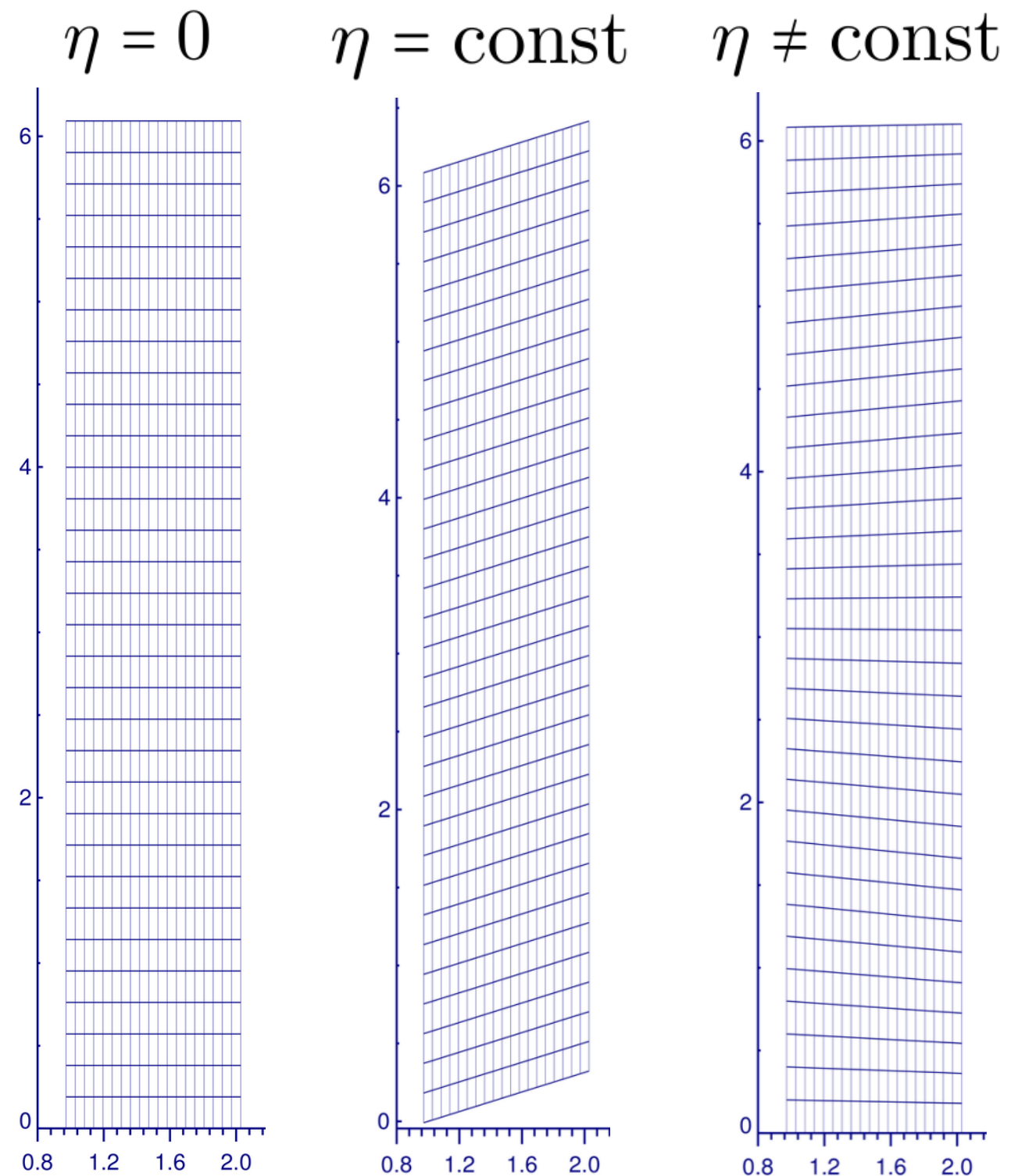
$$z = \phi - \int_{y_0}^y \nu \left( 1 + \int_{\psi_0}^{\psi} \eta \, d\psi \right) dy$$



Can now calculate metric tensors for spatial operators

# Numerical accuracy

- Tested via the method of manufactured solutions<sup>1</sup>
- Nine combination of orthogonalities tested
- Implementation in BOUT++ is 2<sup>nd</sup> order accurate



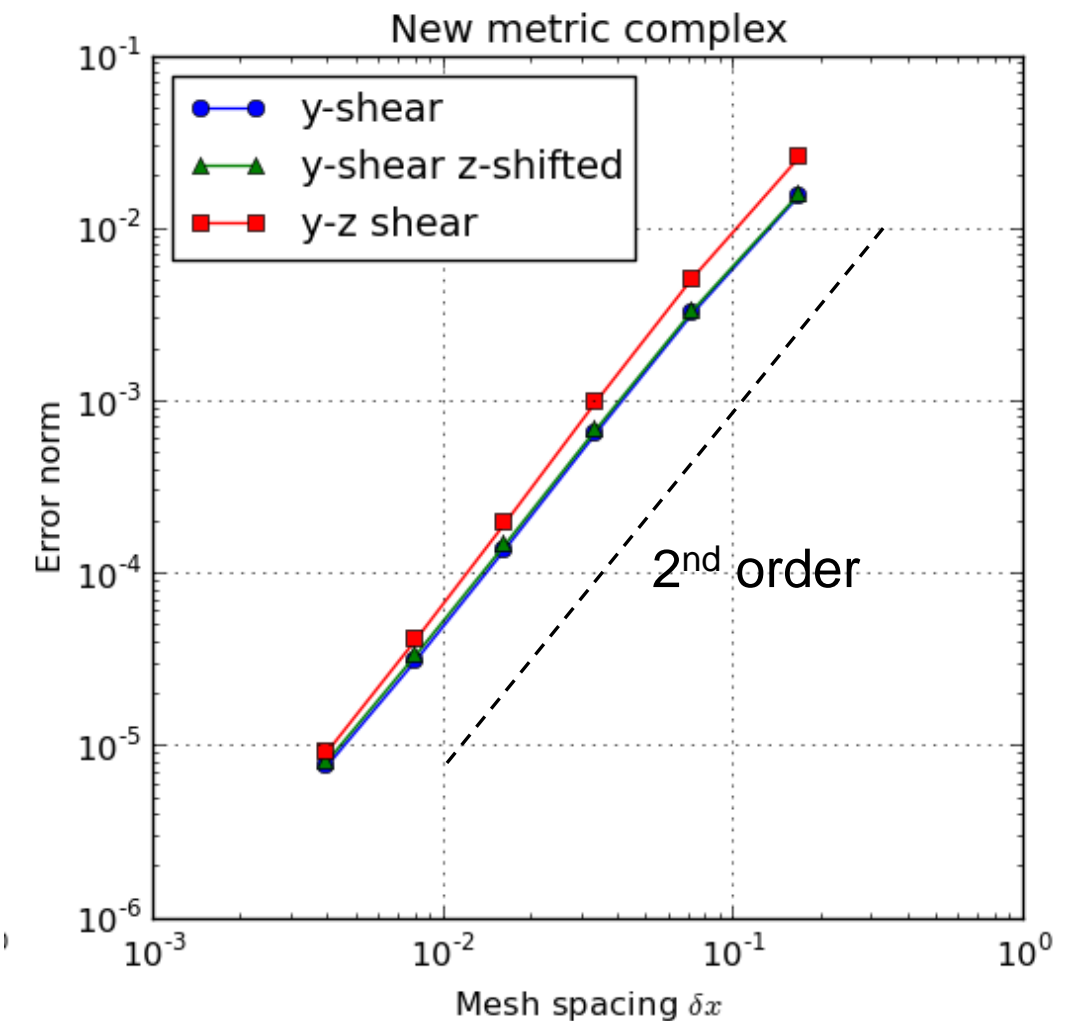
<sup>1</sup> Salari and Knupp, (2000) Tech. Report **SAND2000-1444**

J Leddy *et al* (2017) *Computer Physics Communications*



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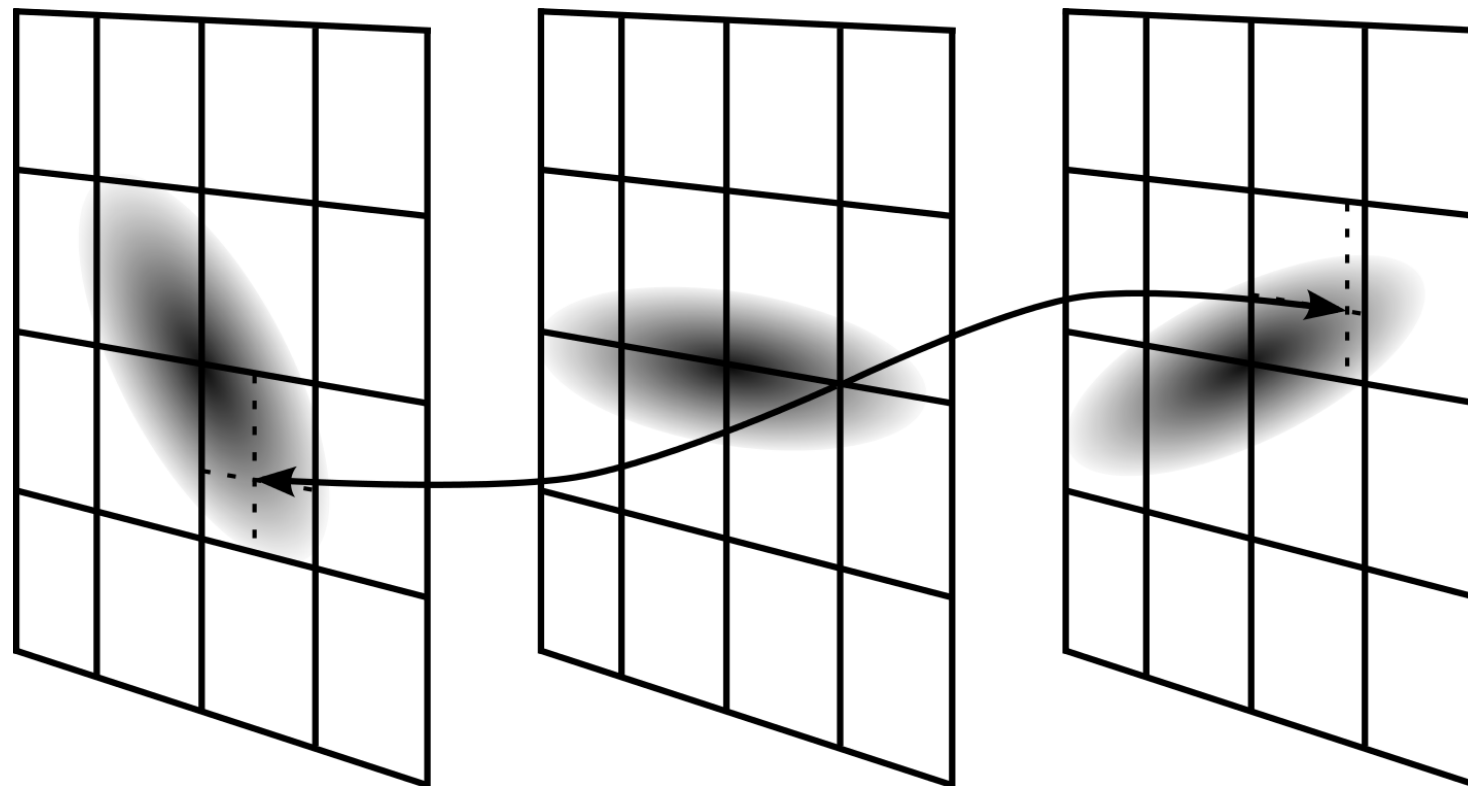
	Orthogonal ( $\eta = 0$ )	Poloidal pitch ( $\eta = \text{const}$ )	Poloidal shear ( $\eta \neq \text{const}$ )
No pitch ( $\nu = 0$ )	2.00	2.14	2.00
Constant pitch ( $\nu = \text{const}$ )	2.02	2.04	2.02
Shear ( $\nu \neq \text{const}$ )	2.14	2.14	2.13

<sup>1</sup> Salari and Knupp, (2000) Tech. Report **SAND2000-1444**  
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# FCI method

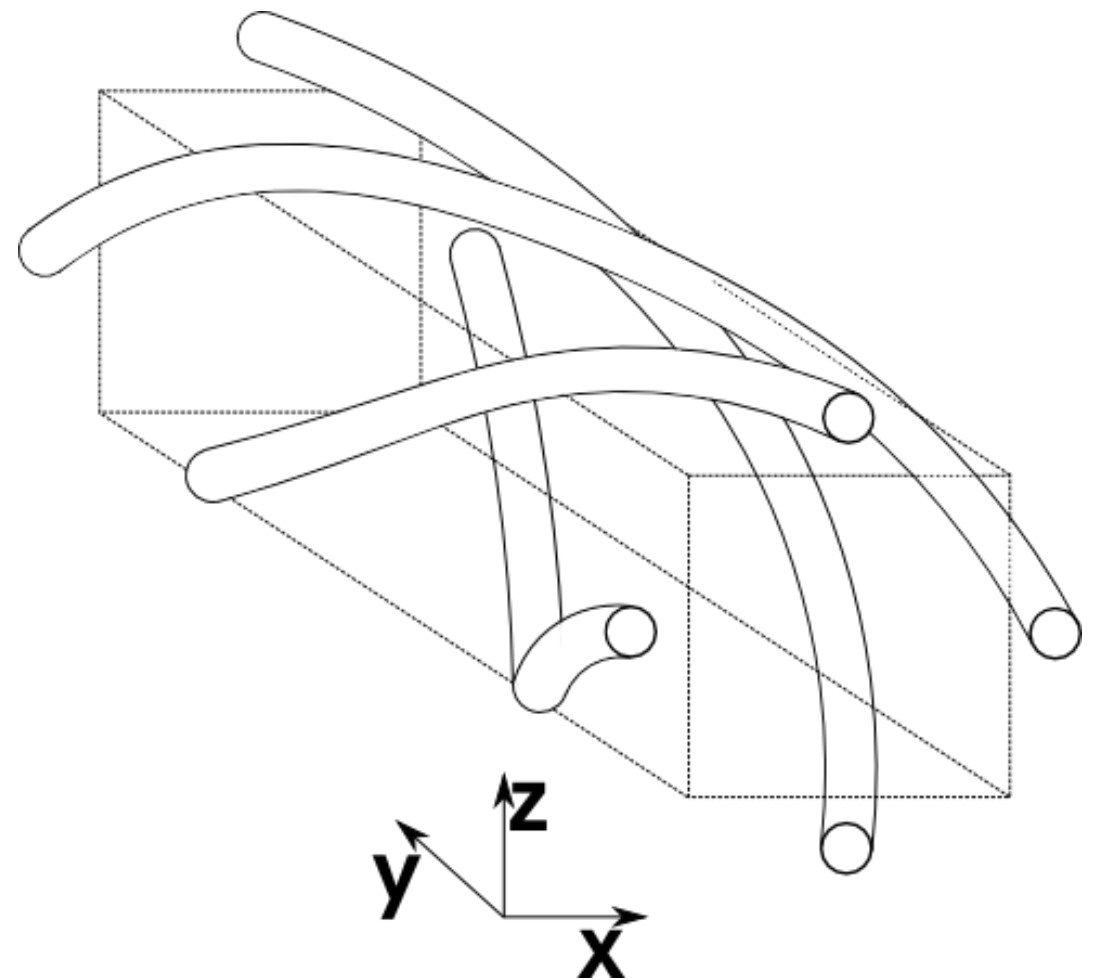
- In irregular and stochastic magnetic fields, having a flux coordinate independent (FCI) system can be preferable
- Cartesian planes – follow field lines and interpolate to perform parallel derivatives
- Benefits:
  - No assumption of flux surfaces
  - Parallel derivative entirely in parallel direction so no singularities in metric



# Straight stellarator test

- As a test of the FCI Method, a straight stellarator was constructed
- Solved parallel diffusion equation to trace flux surfaces
- Inherent perpendicular diffusion reduced to tolerable levels ( $<10^{-8}$ ) for  $\sim 1\text{mm}$  resolution

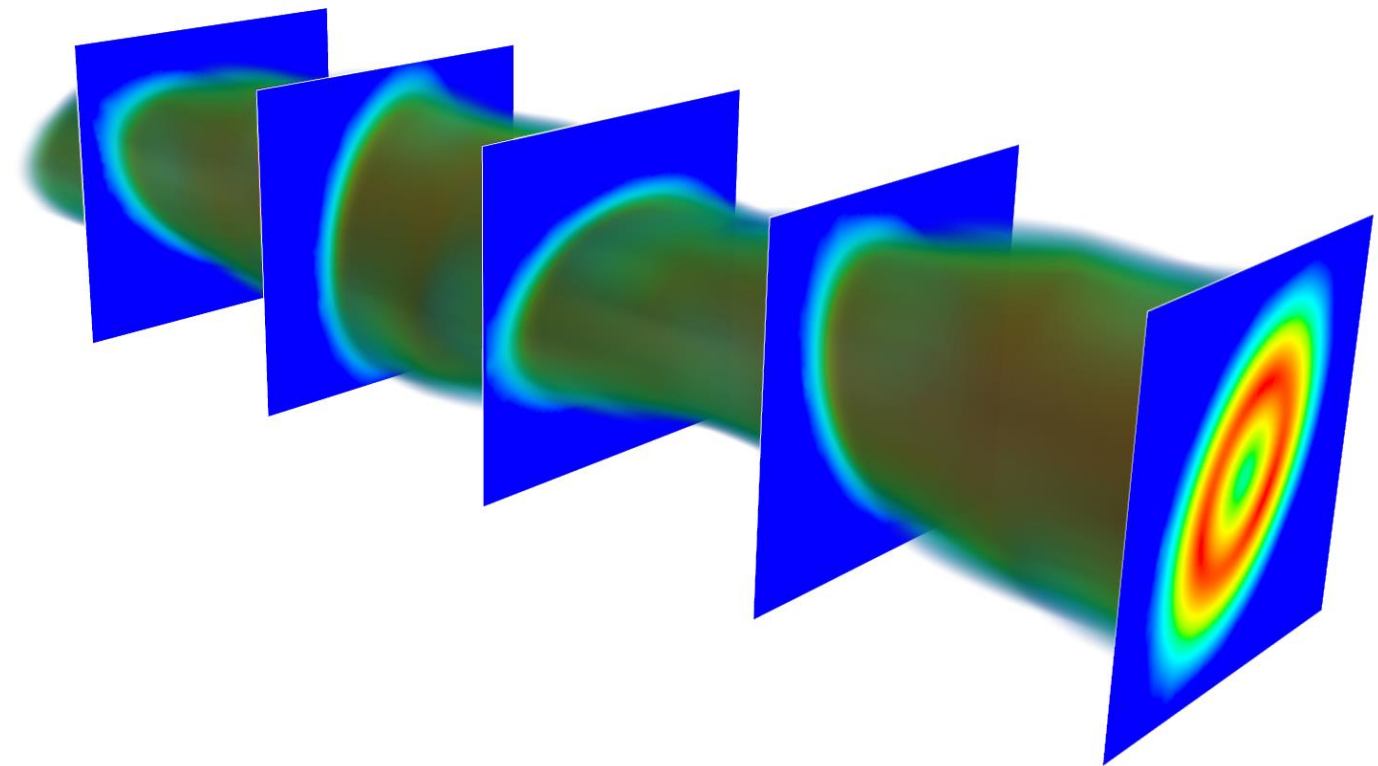
$$d_t(f) = \nabla_{\parallel}^2 f$$



# Straight stellarator test

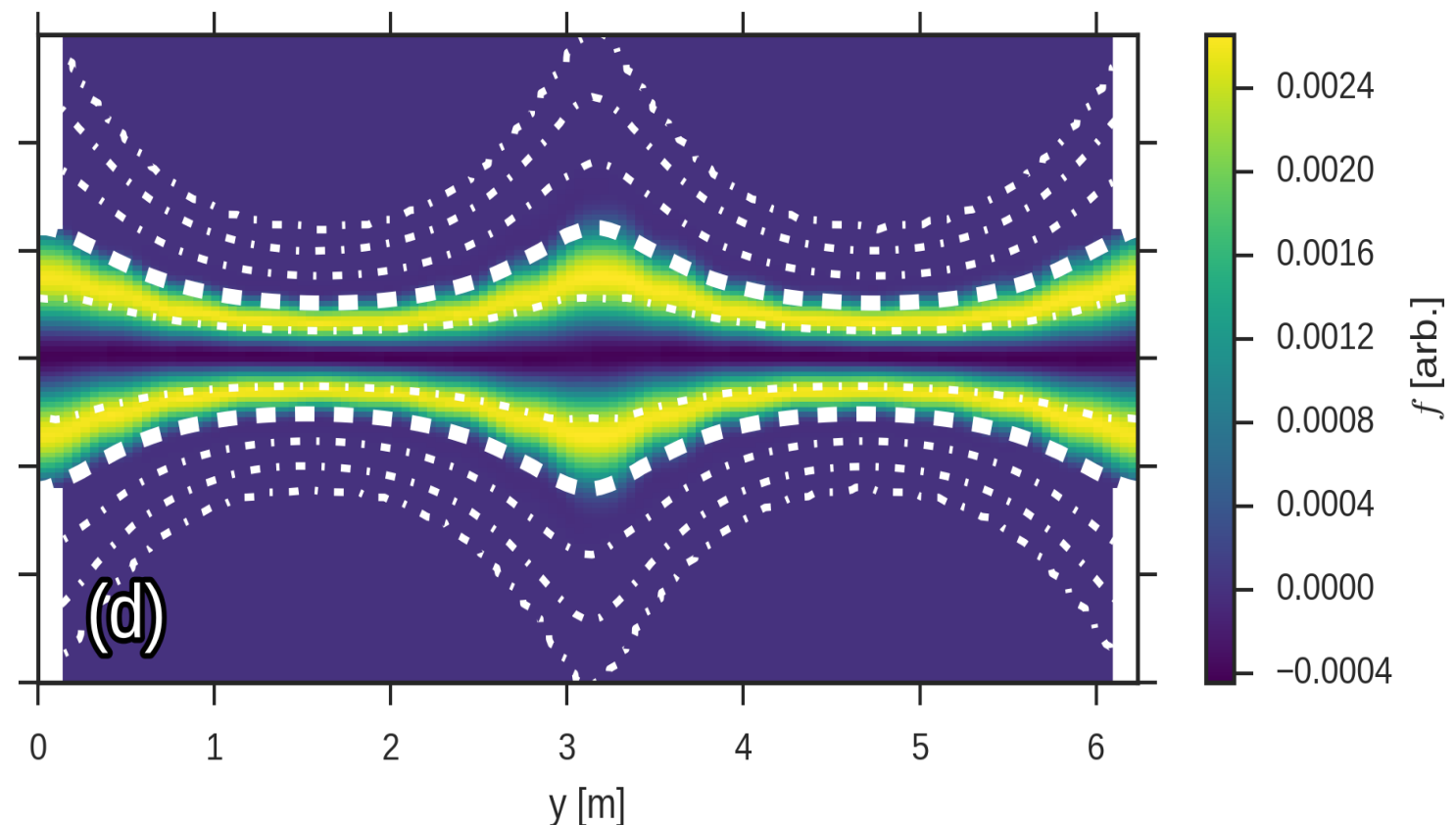
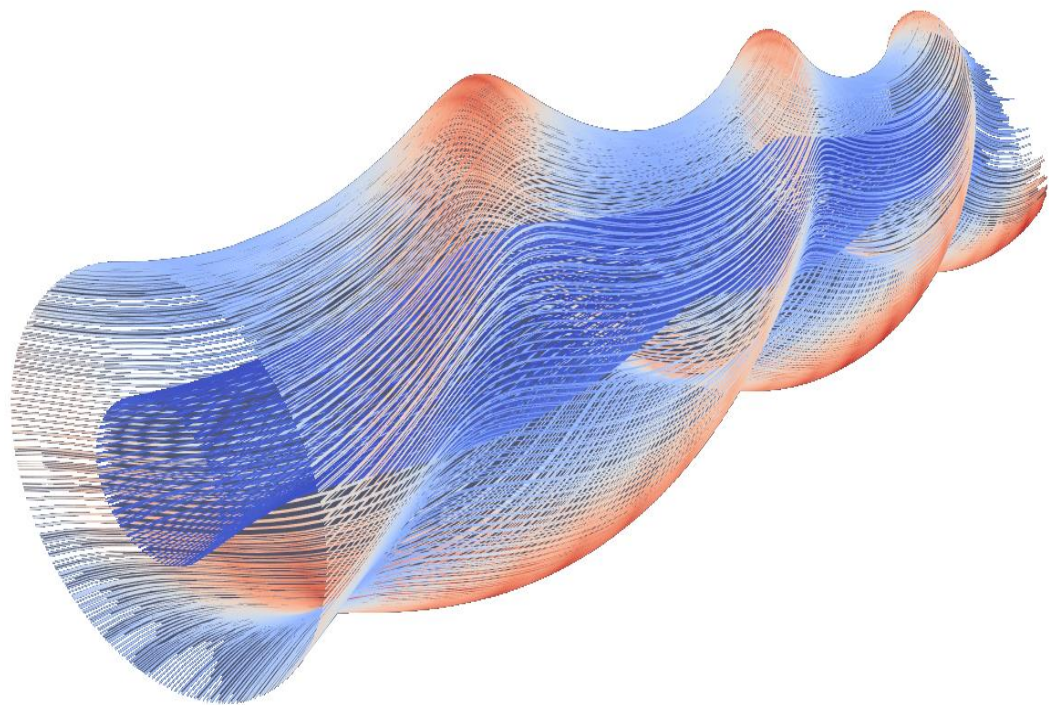
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$$d_t (f) = \nabla_{\parallel}^2 f$$



# Limiter boundary condition

- Recently implemented:
  - Grid generator which takes input from analytic functions, VMEC equilibria, etc.
  - Parallel boundary conditions/poloidal limiters





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# Multi-fluid codes

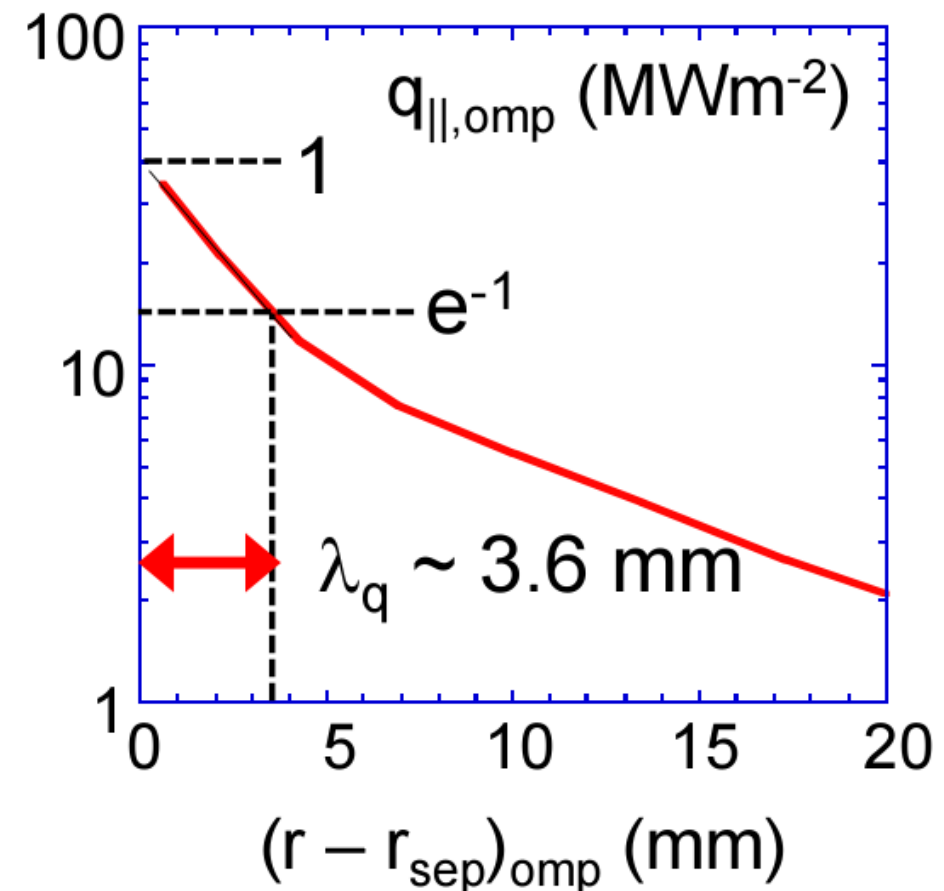
The workhorse of plasma boundary studies  
(e.g SOLPS, EDGE2D, UEDGE, SONIC, ...)

Include detailed physics of  
plasma-wall interaction

- Parallel transport of heat and particles
- Sheath physics
- Neutral gas recycling
- Impurities
- Divertor plates, baffles, ducts, slots, pumps,...

But

Simplified cross-field  
transport



$$D_{\perp} = 0.3 \text{ m}^2\text{s}^{-1}, \chi_{\perp i,e} = 1.0 \text{ m}^2\text{s}^{-1}$$
$$\lambda_q(omp) = 3 - 4 \text{ mm}$$

R.Pitts, IAEA TM on Divertor Concepts (2015)

R Schneider et al. (2006) *Contributions to Plasma Physics*

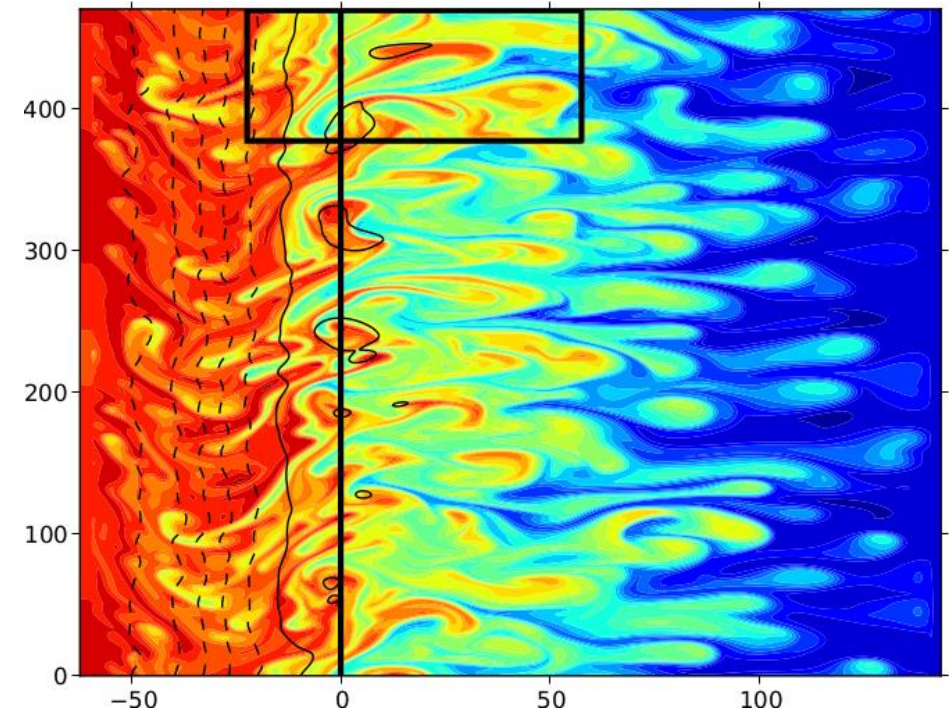
S. Wiesen et al. (2015) *Journal of Nuclear Materials*

X. Bonnin et al. (2016) *Plasma Fusion Research*

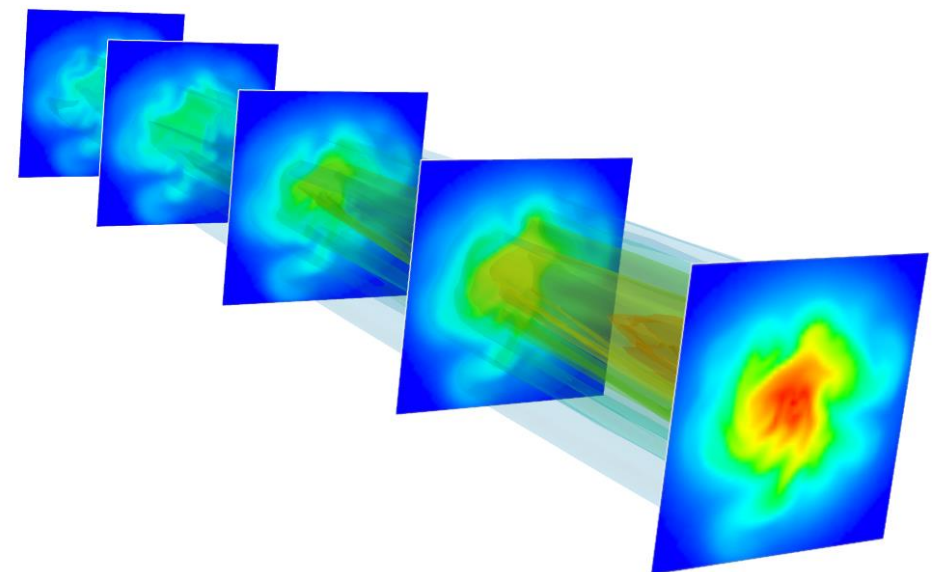
# Turbulence codes

Calculating the turbulent transport requires solving for the time-varying plasma currents and electric fields

- Drift waves, ballooning/interchange instabilities, small-scale structure
- Computationally demanding, timesteps  $<$  ion cyclotron time
- Several codes under development (e.g. GBS, TOKAM-X, HESEL, BOUT++)
- Have not previously included detailed geometry, impurities, neutrals, ...



Dudson, IAEA TM on Plasma Instabilities (2014)

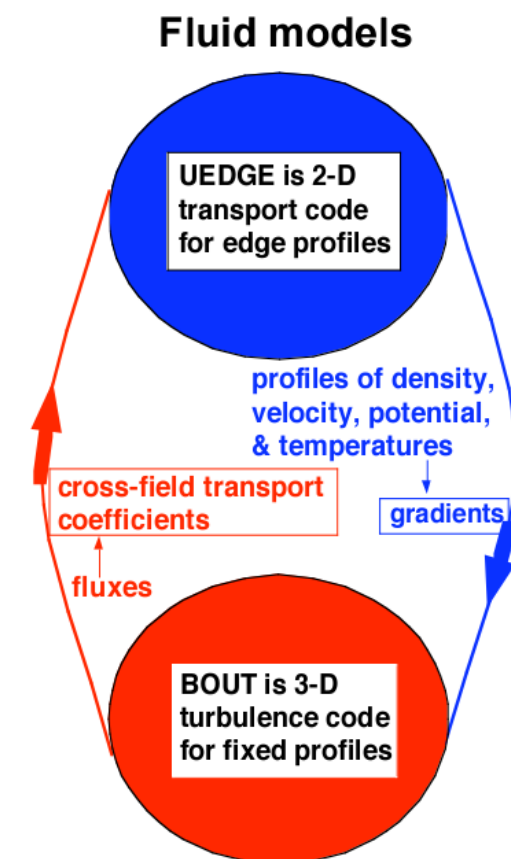
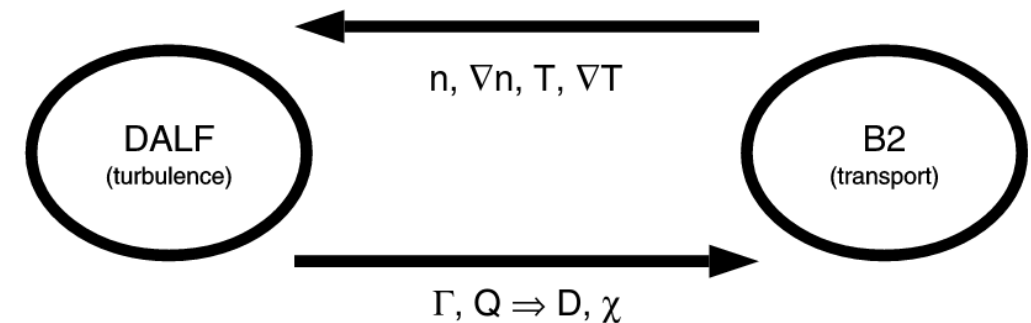


J.Leddy, PSI 2016

# Combining models

- Several attempts to combine transport models with turbulence codes
- Difficulties include
  - Consistency of underlying models
  - Separation of scales
  - Nonlinearity of atomic processes with density, temperature

Here the aim is to combine everything into one simulation, modelling “transport” and turbulence together



R Schneider et al. (2006) *Contrib. Plasma Phys.*

T.D.Rognlien, (2004) ECC meeting

Umansky M V and Rognlien T D (2005) *J. Nucl. Mater.*

F.Guzman et al. (2015) *PPCF*



# The Hermes model

Based on **BOUT++**

<https://github.com/boutproject/hermes>

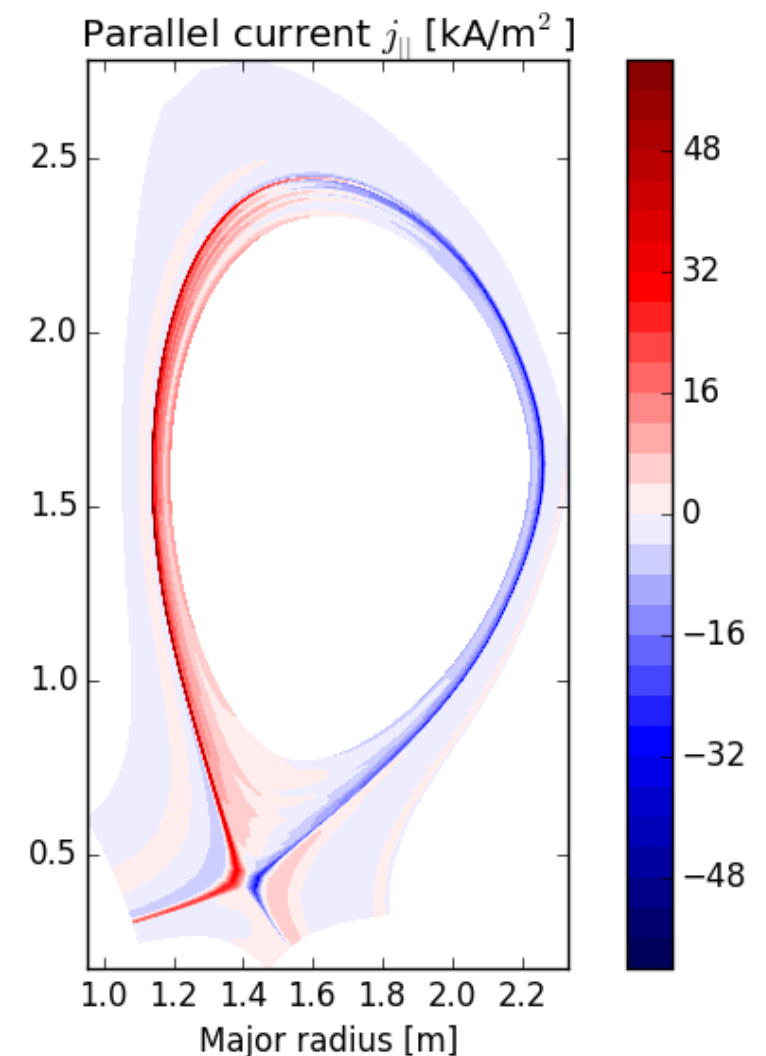
## Current status

- Cold ion drift-fluid model
- Fluid neutrals: Diffusive, full Navier-Stokes, and hybrid models
- New differential operators for particle and energy conservation
- New electric field solver for  $n=0$  mode

Flux-driven edge fluid  
simulations in X-point geometry

## Under development

- Hot ion model
- EIRENE coupling for kinetic neutrals
- Pre-conditioners for faster simulation



# Model equations (1/2)

Evolving (electron) density  $n$ , electron pressure  $p$

$$\frac{\partial n_e}{\partial t} = -\nabla \cdot [n_e (\mathbf{V}_{E \times B} + \mathbf{V}_{mag} + \mathbf{b}v_{||e})] \\ + \nabla \cdot (D_{\perp} \nabla_{\perp} n_e) + S_n$$

$$\frac{3}{2} \frac{\partial p_e}{\partial t} = -\nabla \cdot \left( \frac{3}{2} p_e \mathbf{V}_{E \times B} + \frac{5}{2} p_e \mathbf{b}v_{||e} + p_e \frac{5}{2} \mathbf{V}_{mag} \right) \\ - p_e \nabla \cdot \mathbf{V}_{E \times B} + v_{||e} \partial_{||} p_e + \nabla_{||} (\kappa_{e||} \partial_{||} T_e) \\ + 0.71 \nabla_{||} (T_e j_{||}) - 0.71 j_{||} \partial_{||} T_e + \frac{\nu}{n} j_{||}^2 \\ + \nabla \cdot (D_{\perp} T_e \nabla_{\perp} n_e) + \nabla \cdot (\chi_{\perp} n_e \nabla_{\perp} T_e) + S_p$$

With  $\mathbf{E} \times \mathbf{B}$  and magnetic drifts given by:

$$\mathbf{V}_{E \times B} = \frac{\mathbf{b} \times \nabla \phi}{B} \quad \mathbf{V}_{mag} = -T_e \nabla \times \frac{\mathbf{b}}{B}$$

# Model equations (2/2)

Flows and currents are evolved through the vorticity, ion parallel momentum, and vector potential

$$\begin{aligned} \frac{\partial \omega}{\partial t} = & -\nabla \cdot (\omega \mathbf{V}_{E \times B}) + \nabla_{||} j_{||} - \nabla \cdot (n \mathbf{V}_{mag}) \\ & + \nabla \cdot (\mu_{\perp} \nabla_{\perp} \omega) \end{aligned}$$

Boussinesq approximation

$$\omega = \nabla \cdot \left( \frac{n_0}{B^2} \nabla_{\perp} \phi \right)$$

$$\begin{aligned} \frac{\partial}{\partial t} (n_e v_{||i}) = & -\nabla \cdot [n_e v_{||i} (\mathbf{V}_{E \times B} + \mathbf{b} v_{||i})] - \partial_{||} p_e \\ & + \nabla \cdot (D_{\perp} v_{||i} \nabla_{\perp} n) - F \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial t} \left[ \frac{1}{2} \beta_e \psi - \frac{m_e}{m_i} \frac{j_{||}}{n_e} \right] = & \nu \frac{j_{||}}{n_e} + \partial_{||} \phi - \frac{1}{n_e} \partial_{||} p_e \\ & - 0.71 \partial_{||} T_e \\ & + \frac{m_e}{m_i} (\mathbf{V}_{E \times B} + \mathbf{b} v_{||i}) \cdot \nabla \frac{j_{||}}{n_e} \end{aligned}$$

Finite electron mass,  
electromagnetic

# Conservation properties

- Movement of particles and thermal energy done using finite volumes (fluxes through cell faces), so particles conserved to high precision

Conserved energy

$$E = \int dv \left[ \frac{m_i n_0}{2B^2} |\nabla_{\perp} \phi|^2 + \frac{1}{2} m_i n V_{||i}^2 + \frac{3}{2} p_e + \right. \\ \left. \frac{1}{4} \beta_e |\nabla_{\perp} \psi|^2 + \frac{m_e}{m_i} \frac{1}{2} \frac{j_{||}^2}{n} \right]$$



# Boundary conditions

Interaction with plasma sheath a complex problem. Here relatively simple boundary conditions are used (multiple options in code for boundary conditions)

Ion velocity goes to the sound speed

$$v_{||i} \geq c_s \quad c_s = \sqrt{eT_e/m_i}$$

Conducting wall

$$j_{||} = en_e \left[ v_{||i} - \frac{c_s}{\sqrt{4\pi}} \exp(-\{\phi/T_e\}) \right]$$

Sheath heat flux transmission

$$q = v_{||i} \left( \frac{1}{2} m_i n_e v_{||i}^2 + \frac{5}{2} p_e \right) - \kappa_{||e} \partial_{||} T_e = \gamma_s n_e T_e c_s$$

with  $\gamma_s = 6.5$

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P C Stangeby. (2000) *The Plasma Boundary of Magnetic Fusion Devices*

J Loizu, et al. (2012) *Physics of Plasmas*

M U Siddiqui et al. (2016) *Physics of Plasmas*

# New solver for electric potential

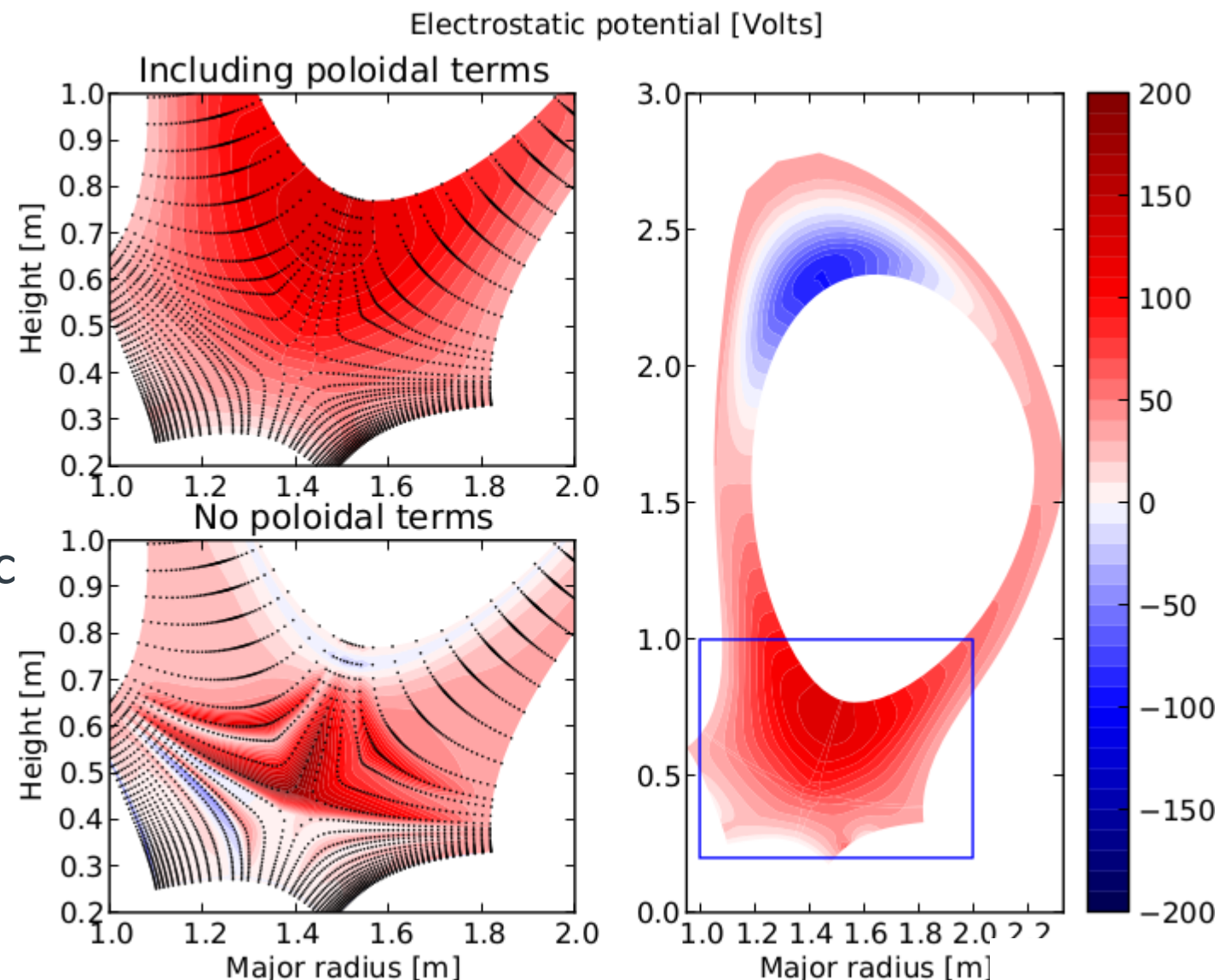
To calculate electrostatic potential we invert the vorticity:

$$\nabla \cdot \left( \frac{m_i n}{B^2} \nabla_{\perp} \phi \right) = \frac{1}{J} \frac{\partial}{\partial u^i} \left( J \frac{m_i n}{B^2} g^{ij} (\nabla_{\perp} \phi)_j \right)$$

For low-n modes the poloidal terms become important

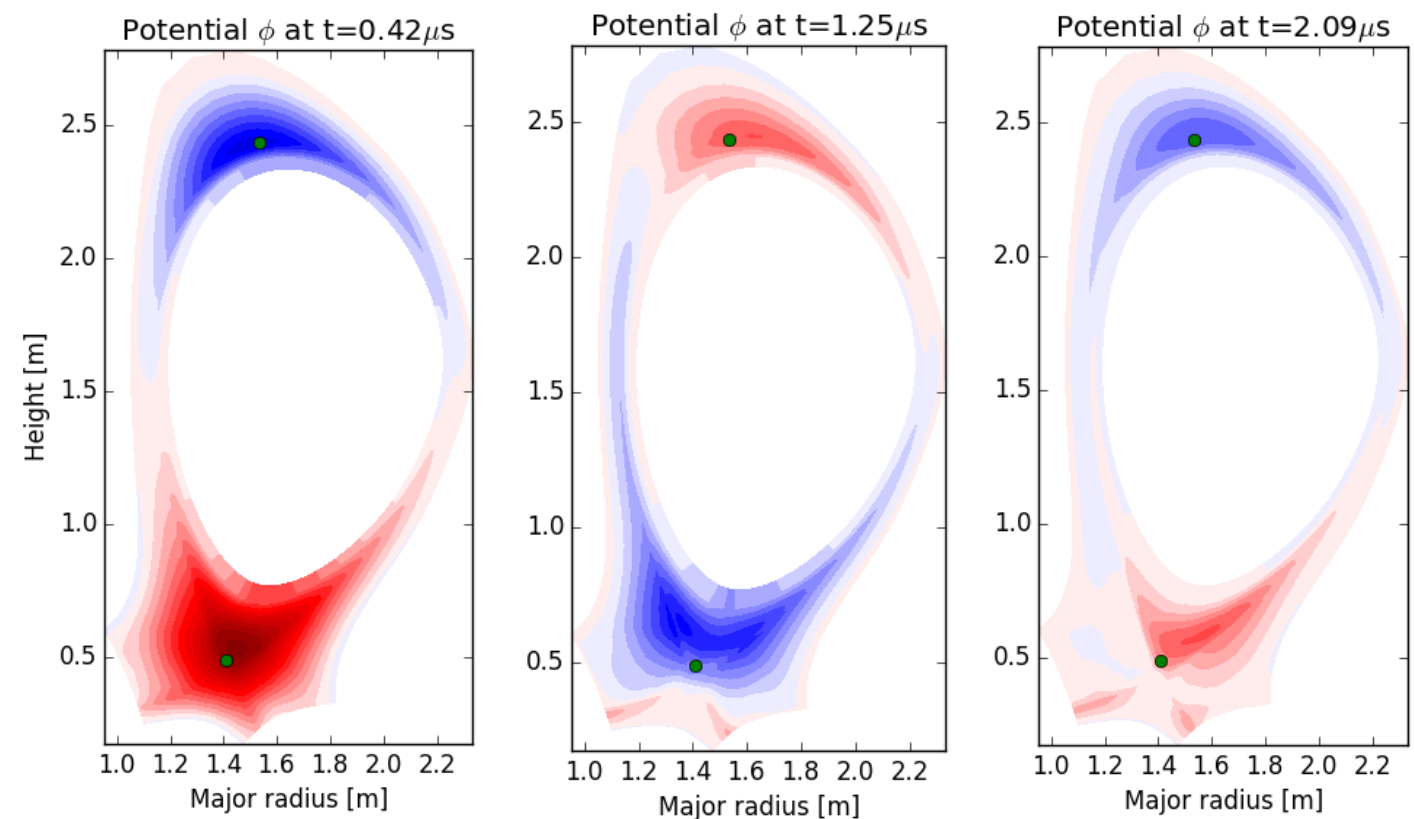
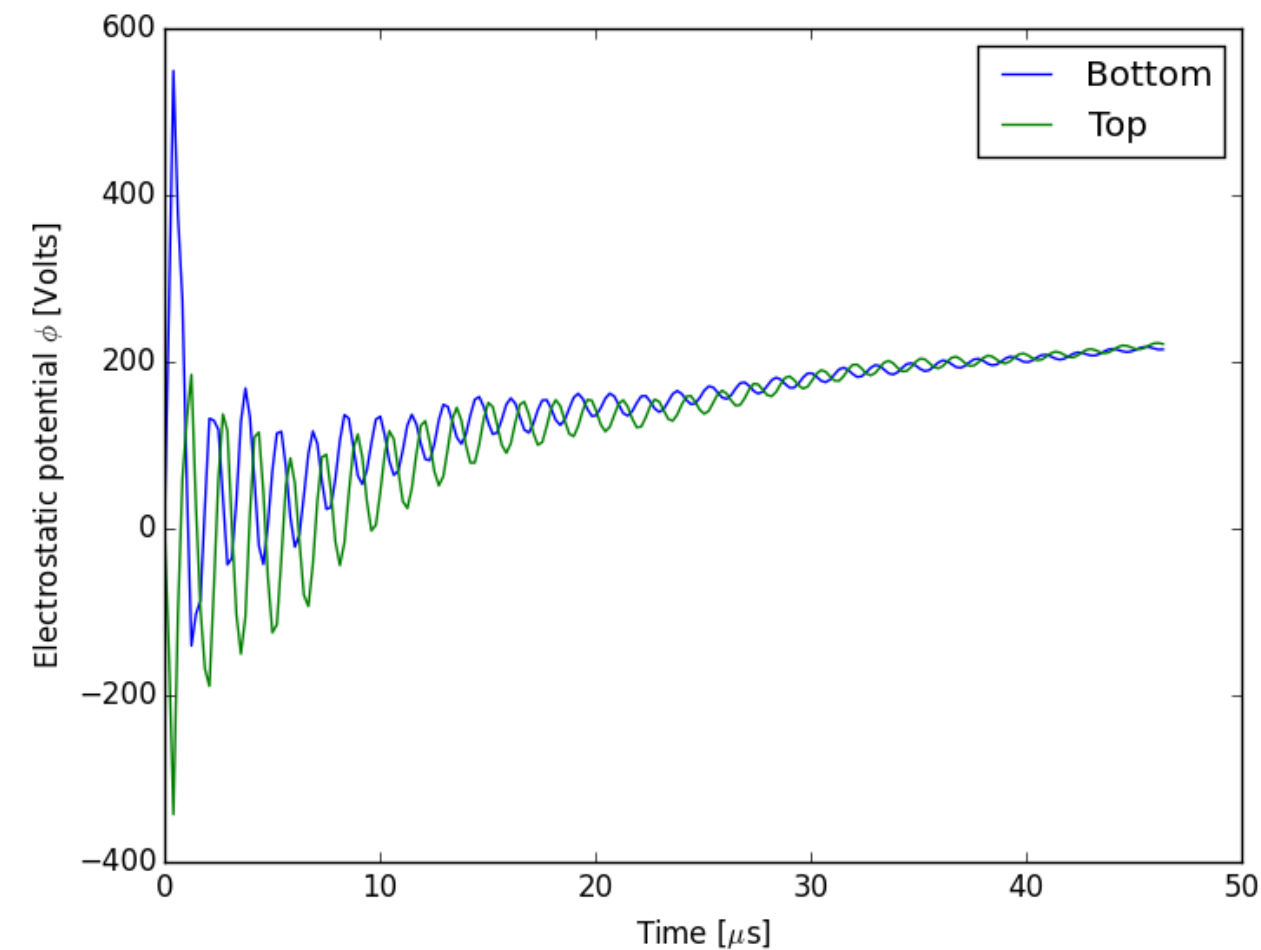
Around the X-point unphysical oscillations occur if poloidal terms are neglected

→ New solver implemented using PETSc for axisymmetric (n=0) component



# Successfully evolve $n=0$ potential

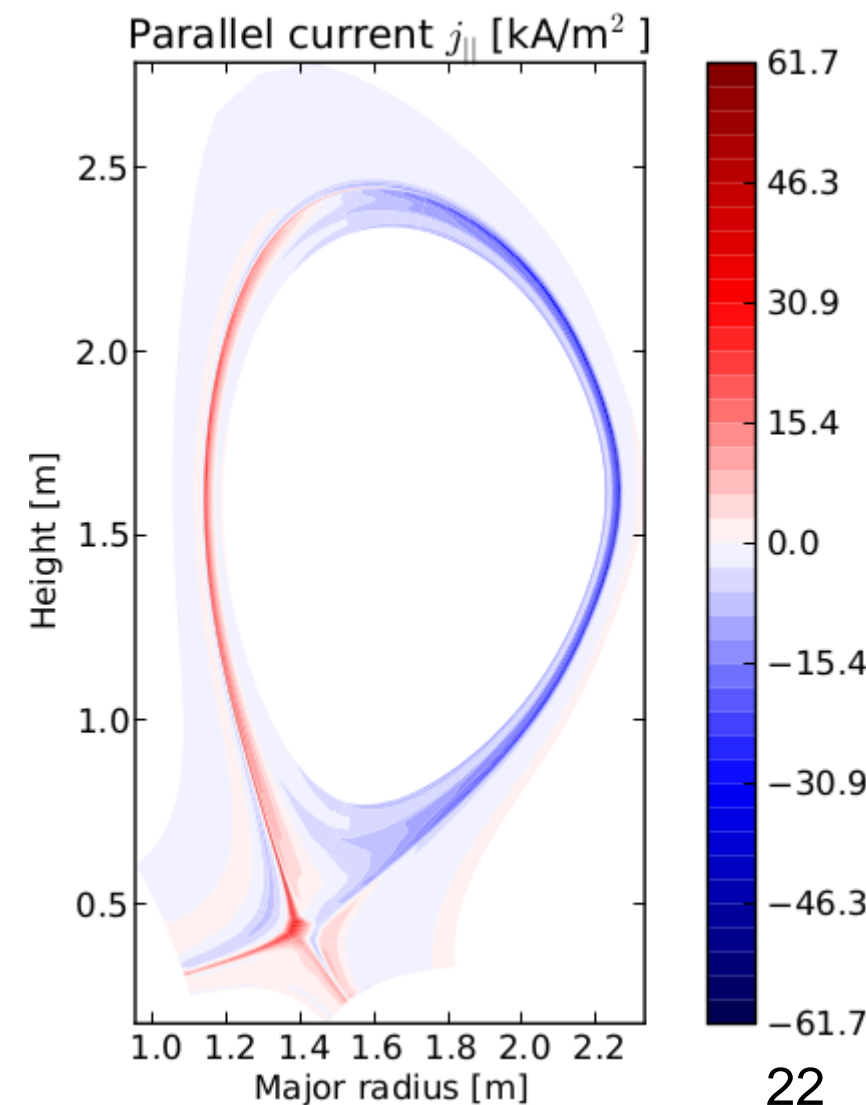
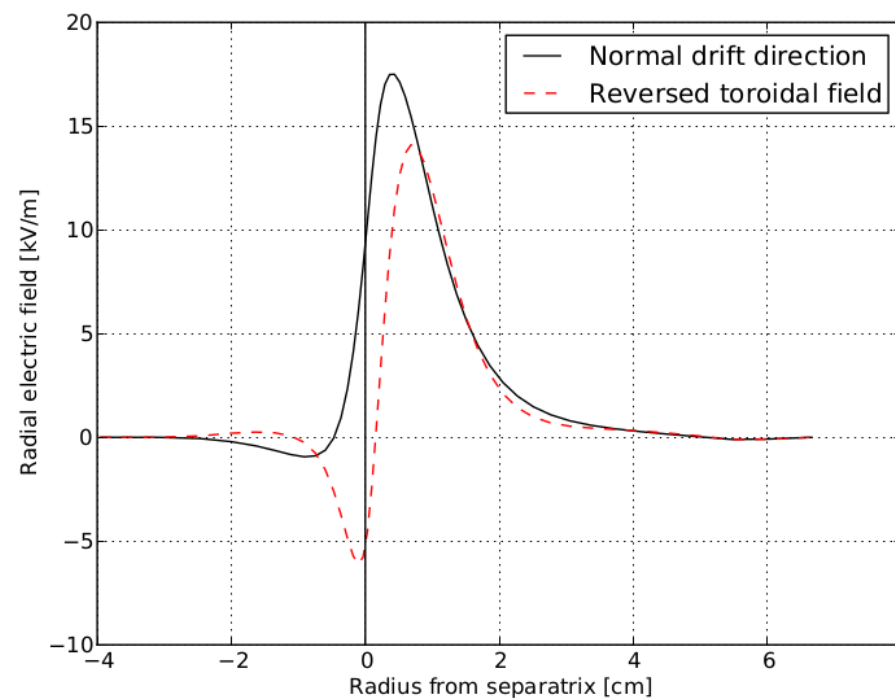
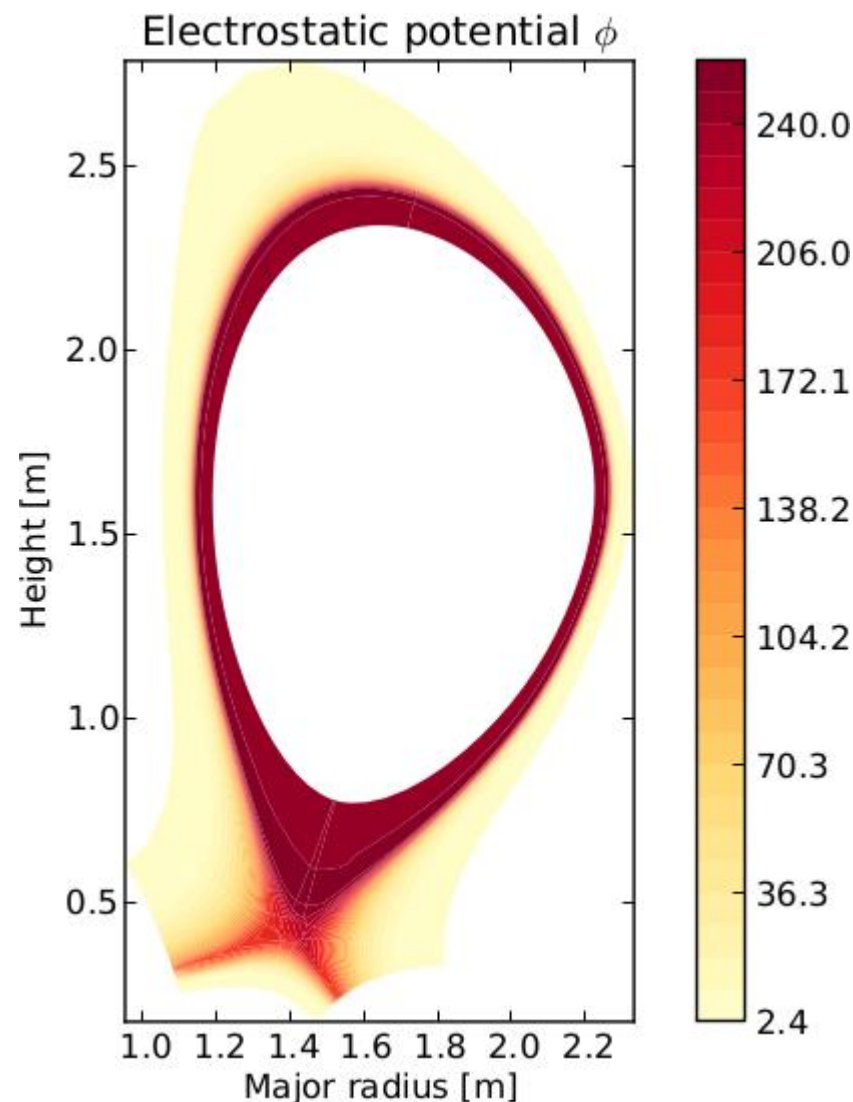
- Initial Alfvénic oscillations  $f \sim 500$  kHz damp on  $\sim 20 \mu\text{s}$  timescale



→ First time this has been possible with BOUT / BOUT++ in X-point geometry

# Radial electric field

- Quasi-steady state has large radial electric field in SOL, driven by sheath and parallel electron force balance
- Reversing toroidal field modifies  $E_r$  near separatrix
- Poloidal rotation sensitive to subtle effects, missing e.g. ion pressure





# Neutral gas model (1/2)

Neutral gas is modelled as a fluid

$$\frac{\partial n_n}{\partial t} = -\nabla \cdot [\mathbf{V}_n n_n] + S$$
$$\frac{\partial}{\partial t} \left( \frac{3}{2} p_n \right) = -\nabla \cdot \mathbf{q}_n + \mathbf{V}_n \cdot \nabla p_n + E$$

$$\mathbf{q}_n = \frac{5}{2} p_n \mathbf{V}_n - \kappa_n \nabla T_n$$

Where  $S$  and  $E$  represent transfer of particles and energy between plasma and neutrals.

- Long mean free path of neutrals means Monte-Carlo treatment necessary in many cases
- Molecules not included. Can be important in high density regions
- Fluid model allows qualitative analysis and interpretation

# Neutral gas model (2/2)

Model follows approach used in UEDGE

- Parallel to the magnetic field the neutral momentum equation is:

$$\frac{\partial}{\partial t} (m_i n_n V_{||n}) = -\nabla \cdot [m_i n_n V_{||n} \mathbf{b} V_{||n}] - \partial_{||} p_n + F$$

- Perpendicular to the magnetic field, neglect neutral inertia, and balance neutral pressure against friction:

$$\mathbf{F}_{\perp} \simeq -\nu \mathbf{V}_{n\perp}$$

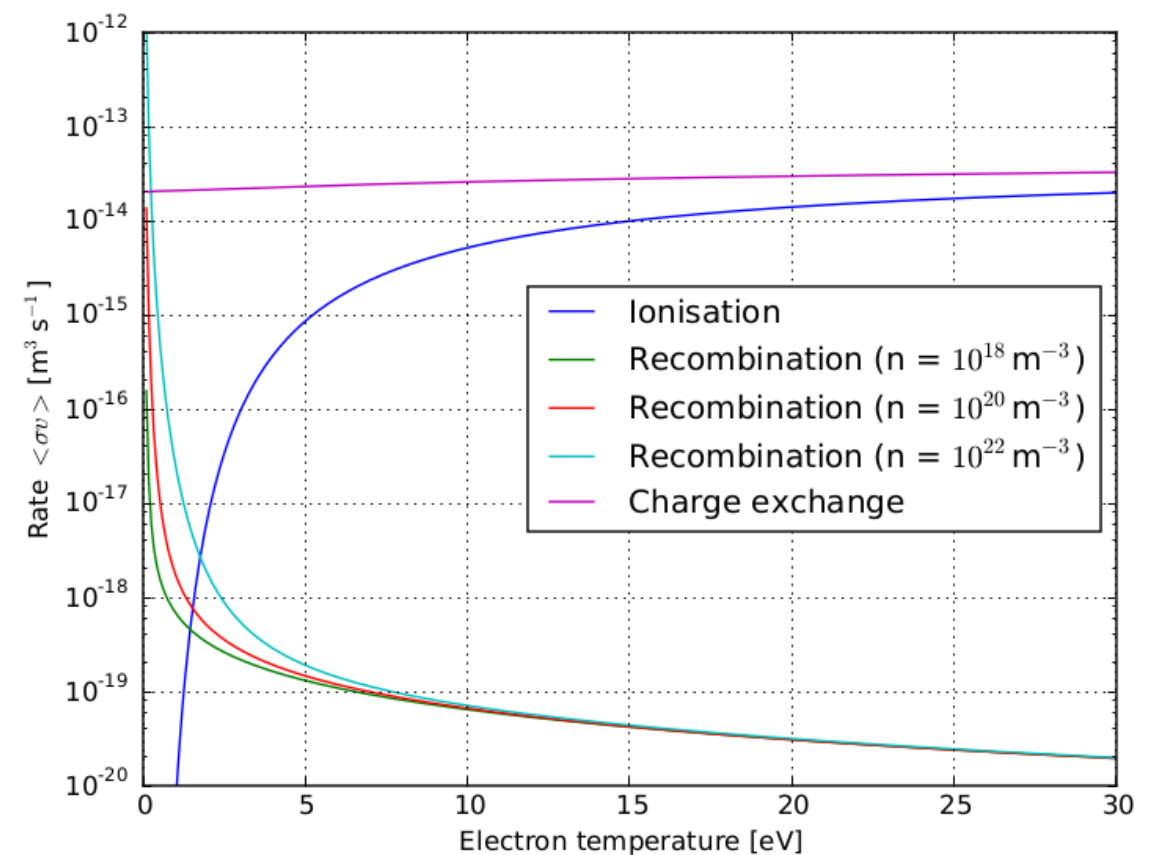
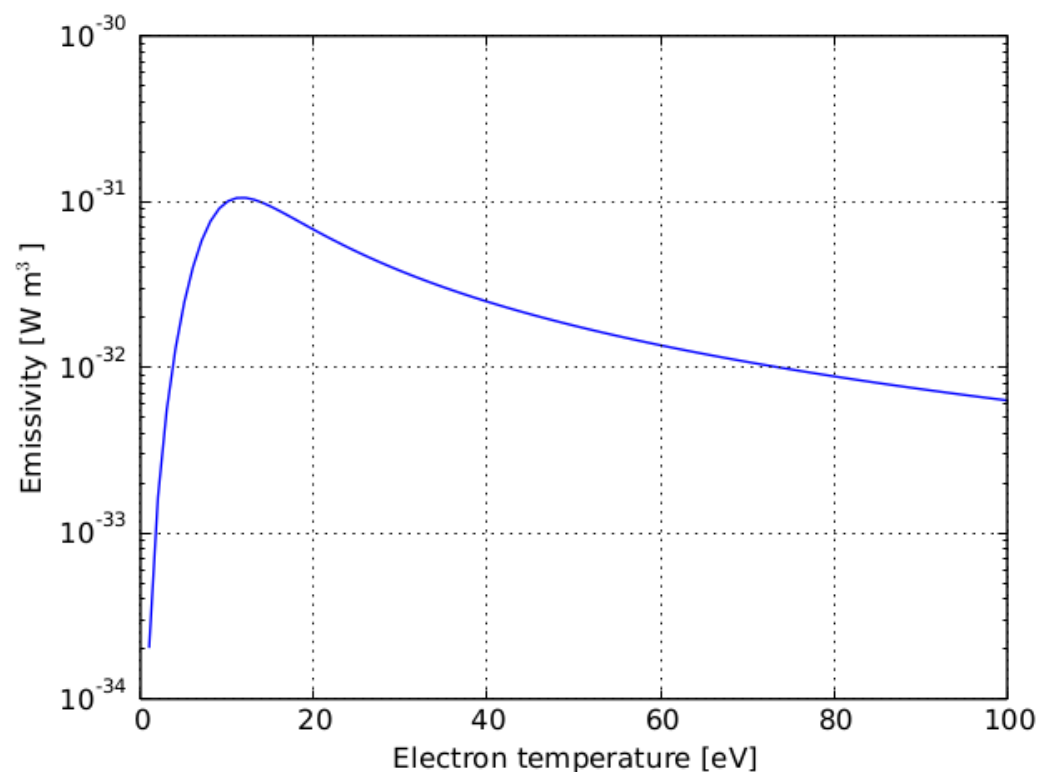
$$\mathbf{V}_{n\perp} = -\frac{1}{\nu} \nabla_{\perp} p_n$$

$$\nu = \nu_{cx} + \nu_{iz} + \nu_{nn}$$

Collision rate = Charge exchange,  
ionisation, neutral-neutral

# Atomic physics

- No molecular processes, only atoms evolved
- Simple semi-analytic fits used for atomic processes: Ionisation, recombination and charge exchange
- Provide source/sinks of particles, momentum and energy



- Carbon impurity included using fixed ion fraction (1% typically)
- Analytic radiation curve from Hutchinson thermal fronts paper

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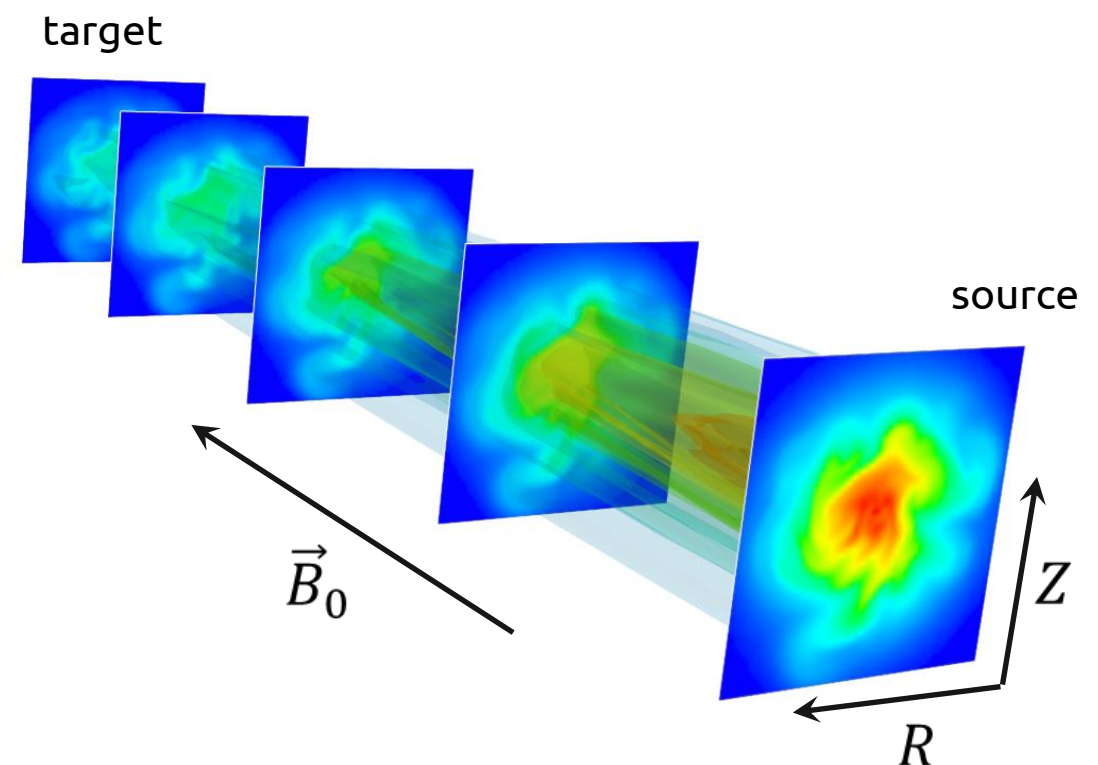
- DIII-D

# Combining turbulence + neutrals

Turbulence + neutrals, linear geometry

- Linear devices have simple geometries, making them a nice test-bed for plasma-neutral interaction
- We have simulated a small Magnum-PSI sized device with the following parameters:

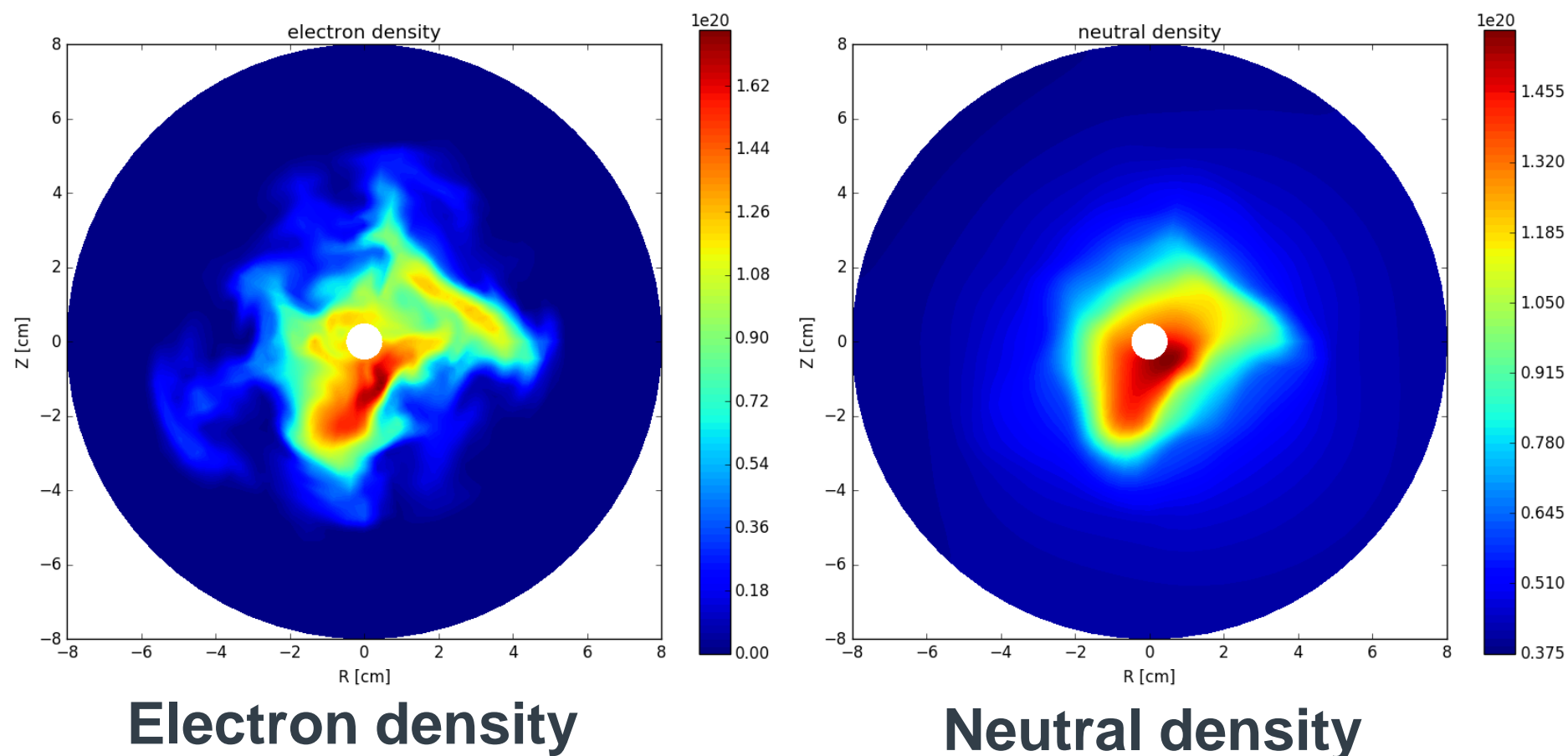
Magnetic field	0.15 T
Length	1.2 m
Radius	10 cm





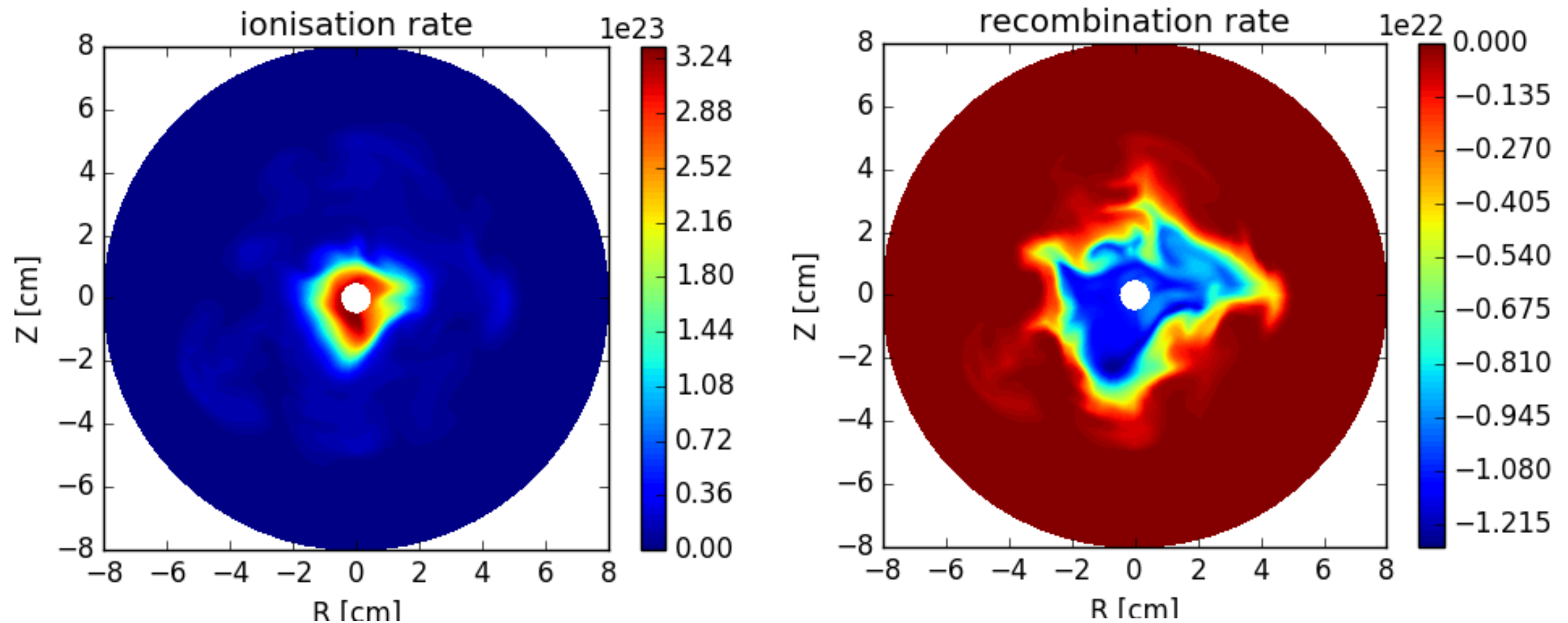
# Combining turbulence + neutrals

- Strong turbulence leads to significant modification of profiles (aided by insulating sheath boundary condition)
- Peak density off-axis at times
- Affects interaction with neutrals: only sources of neutrals are recycling at the target, and volume recombination



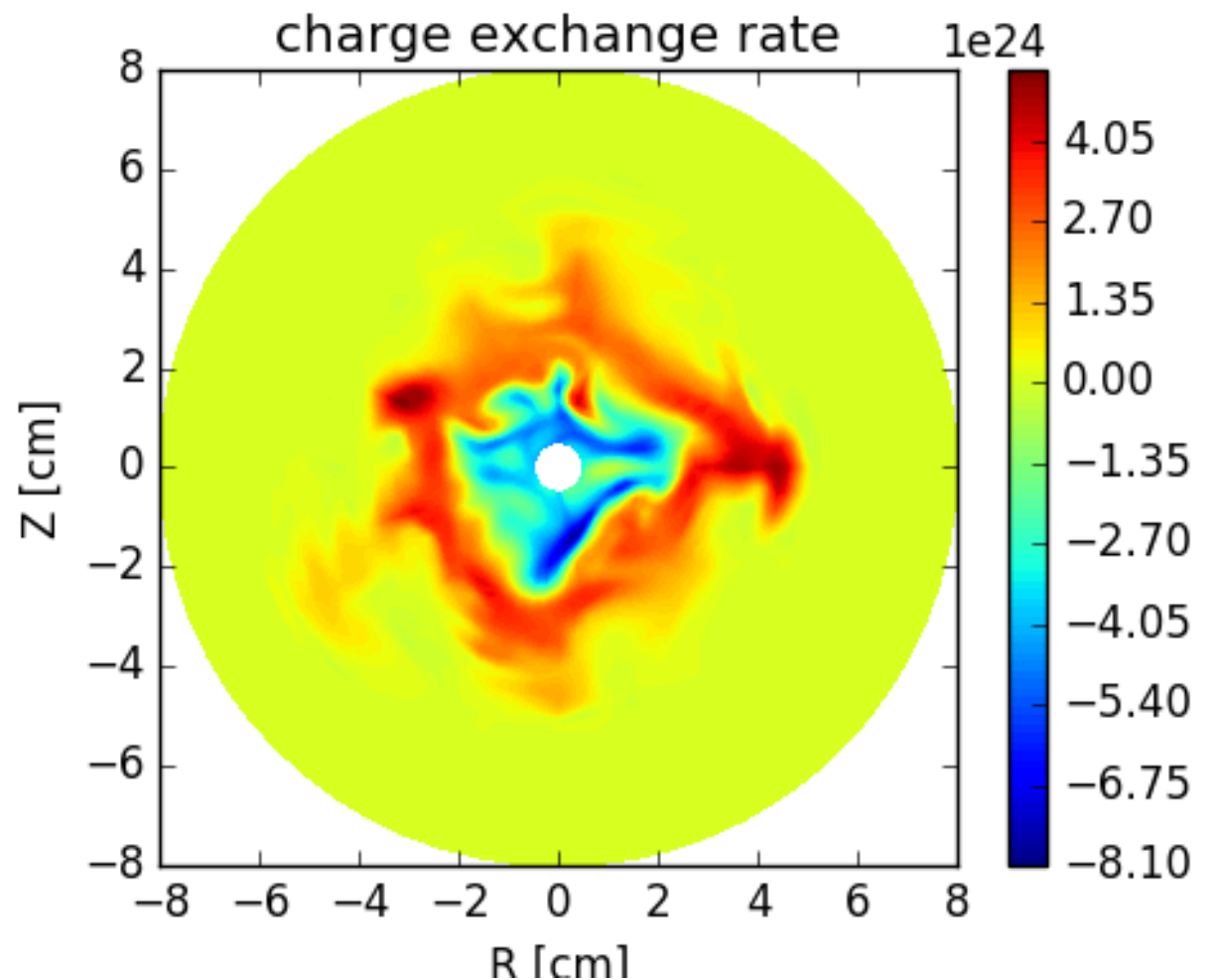
# Particle source/sinks

- Ionisation mainly occurs in highest density and temperature regions of the plasma (centre of eddies)
- Recombination is localised to the high density but low temperature regions (edge of the eddies)

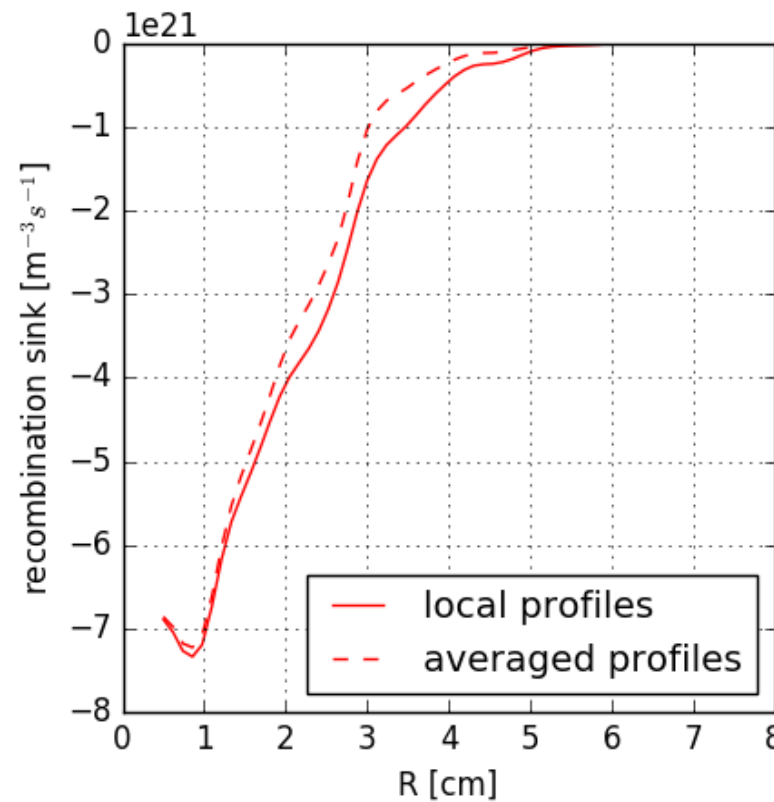
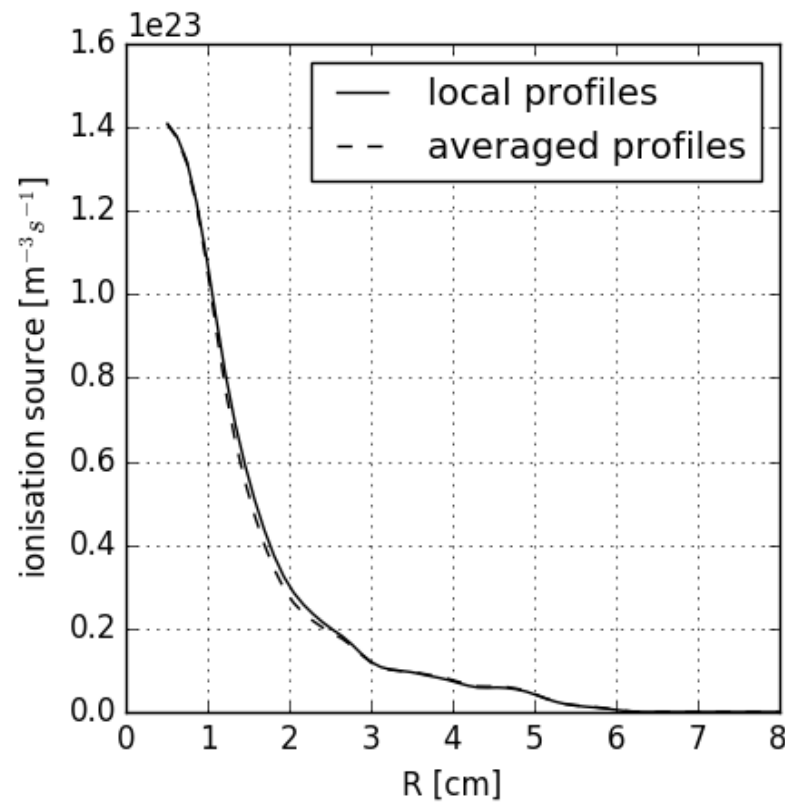


# Charge-exchange

- Significant energy is only removed where the temperature difference is greatest ( $T_e - T_n$ )
- Energy removed from plasma in centre (hottest region)
- Energy transferred to plasma in the edge, where  $T_n > T_e$
- Note: cold ion model, so electron temperature used for atomic processes

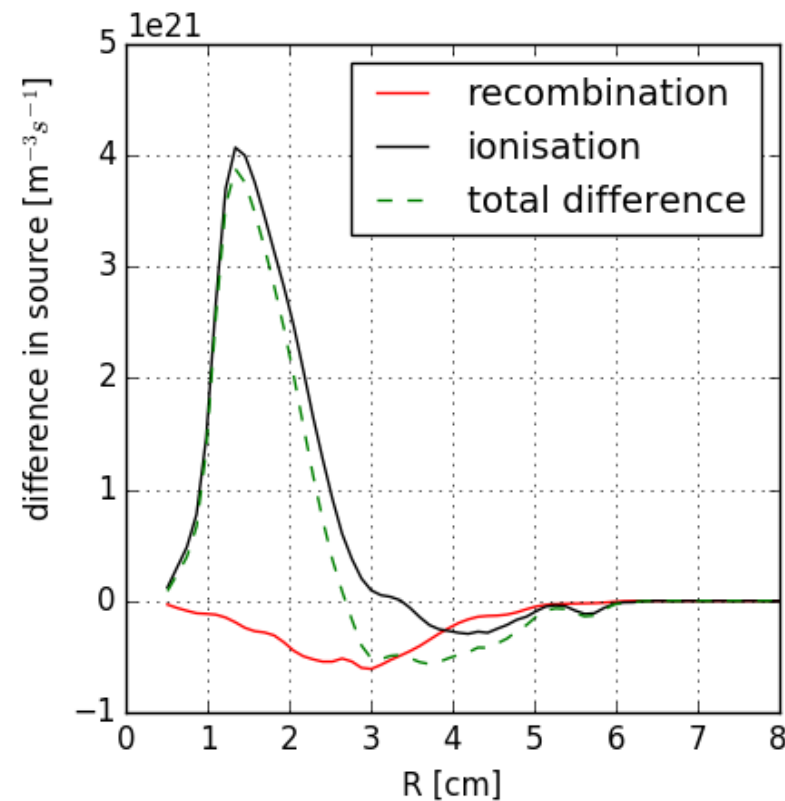


# Effect of fluctuations



Local profiles  
 $\frac{n_e n_n \langle \sigma v \rangle (T_e)}{\bar{n}_e \bar{n}_n \langle \sigma v \rangle (\bar{T}_e)}$

Axially-averaged profiles  
 $\bar{n}_e \bar{n}_n \langle \sigma v \rangle (\bar{T}_e)$





- Averaged over  $8000 \omega_{ci}^{-1}$  ( $\sim 0.17$ ms)
- Consistently higher neutral source with turbulence than without
- Difference in source/sinks peaks off-axis
- $\sim 10\%$  max difference in ionisation,  $\sim 50\%$  max difference in recombination

# Including drifts is challenging


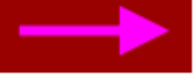

- Balance of diamagnetic, parallel and polarisation currents
- Sheath currents at divertor
- Electric fields modify flows, edge asymmetries

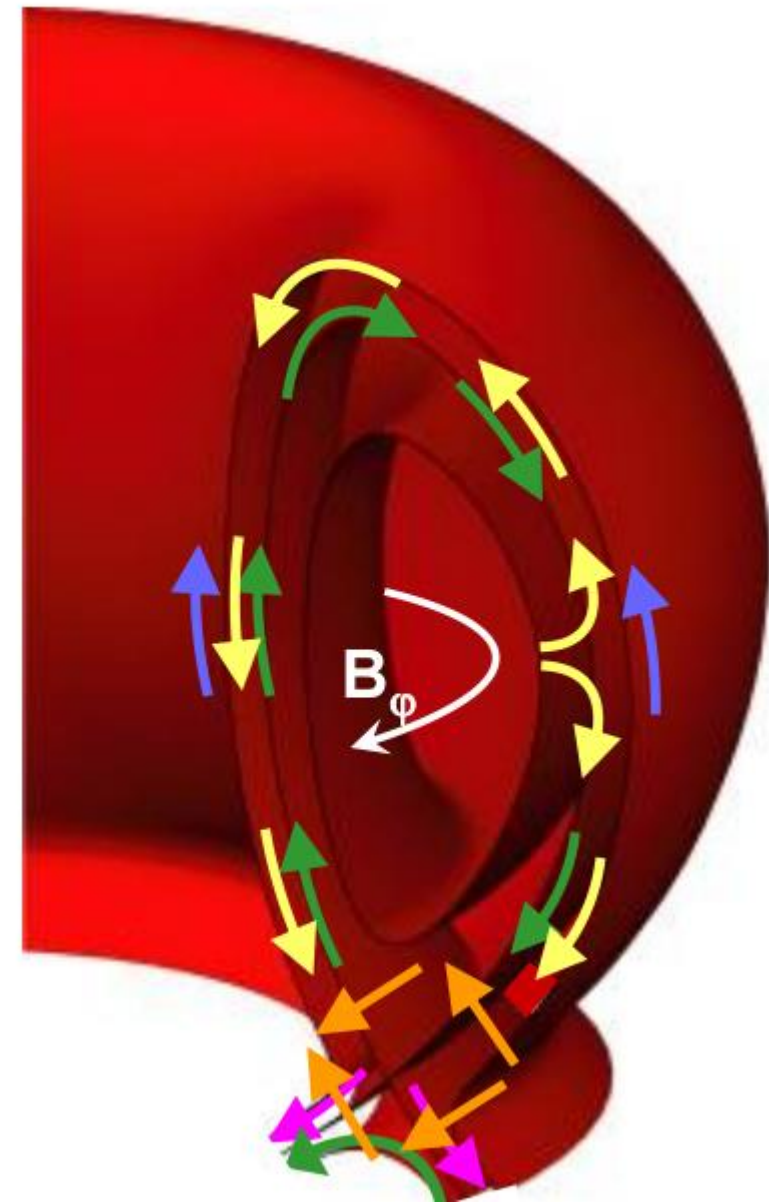
Introduces rapid timescales:  
Alfven waves, electron parallel dynamics

- Typically reduces timestep by factor of  $\sim 10$
- Can lead to numerical instabilities

$E_r \times B, \nabla p \times B$	
$E_\theta \times B$	

**Poloidal**

Pfirsch-Schlüter	
Divertor sink	
$\perp$ transport driven	

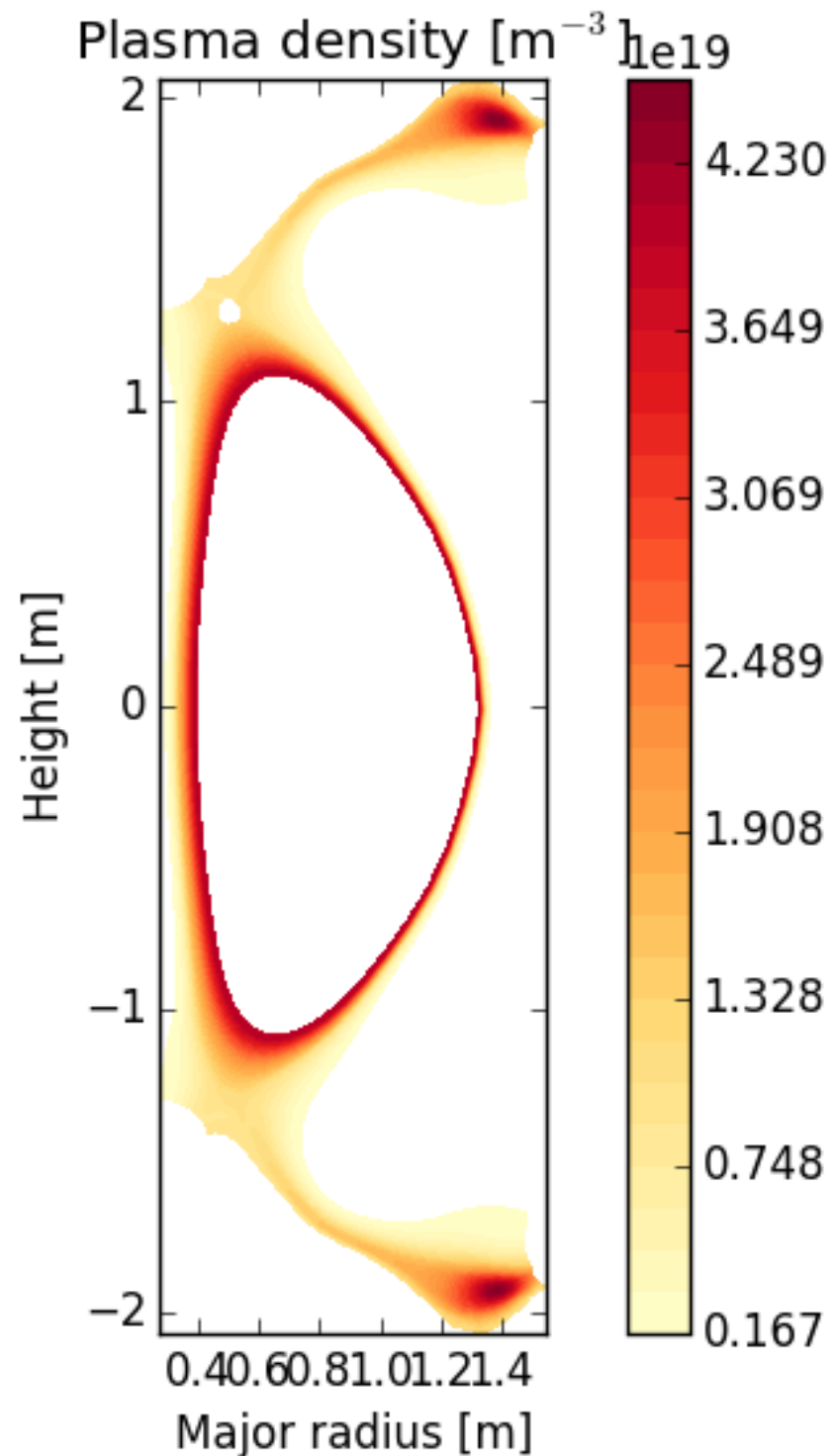


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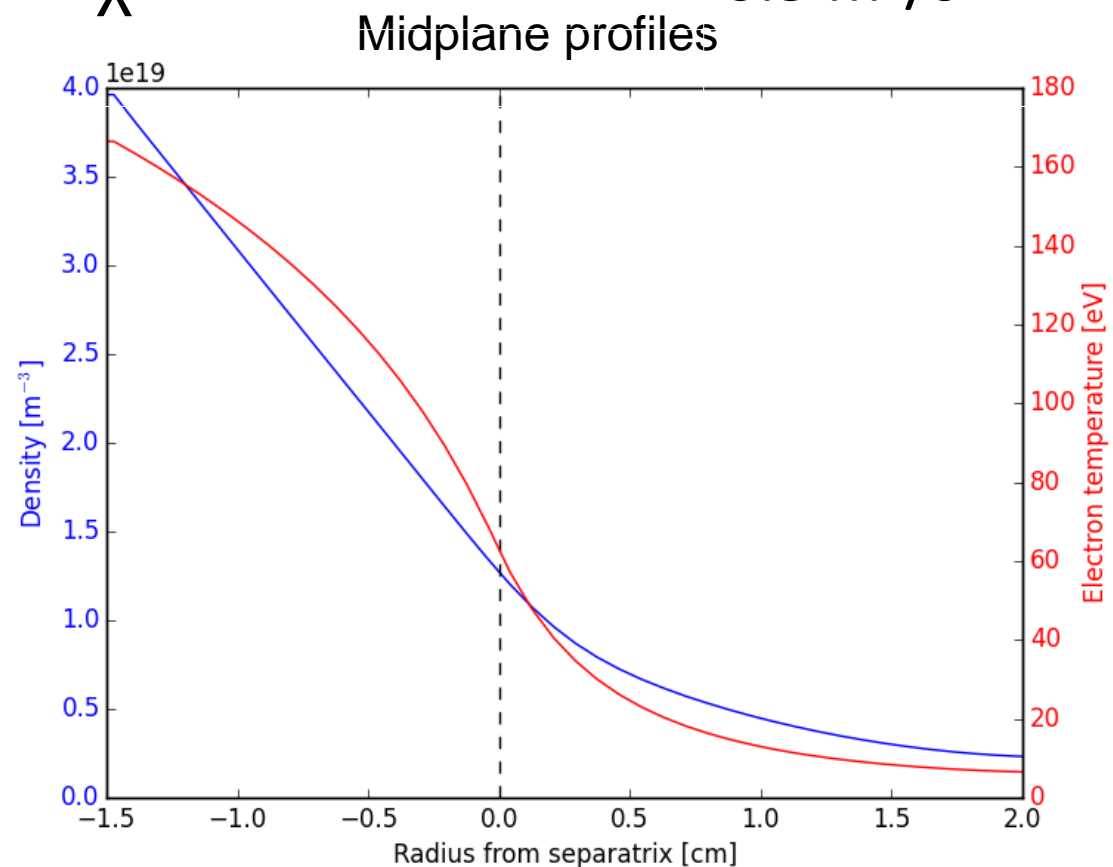


# MAST-Upgrade simulations

Axisymmetric fluid simulation: No electric fields, no turbulence

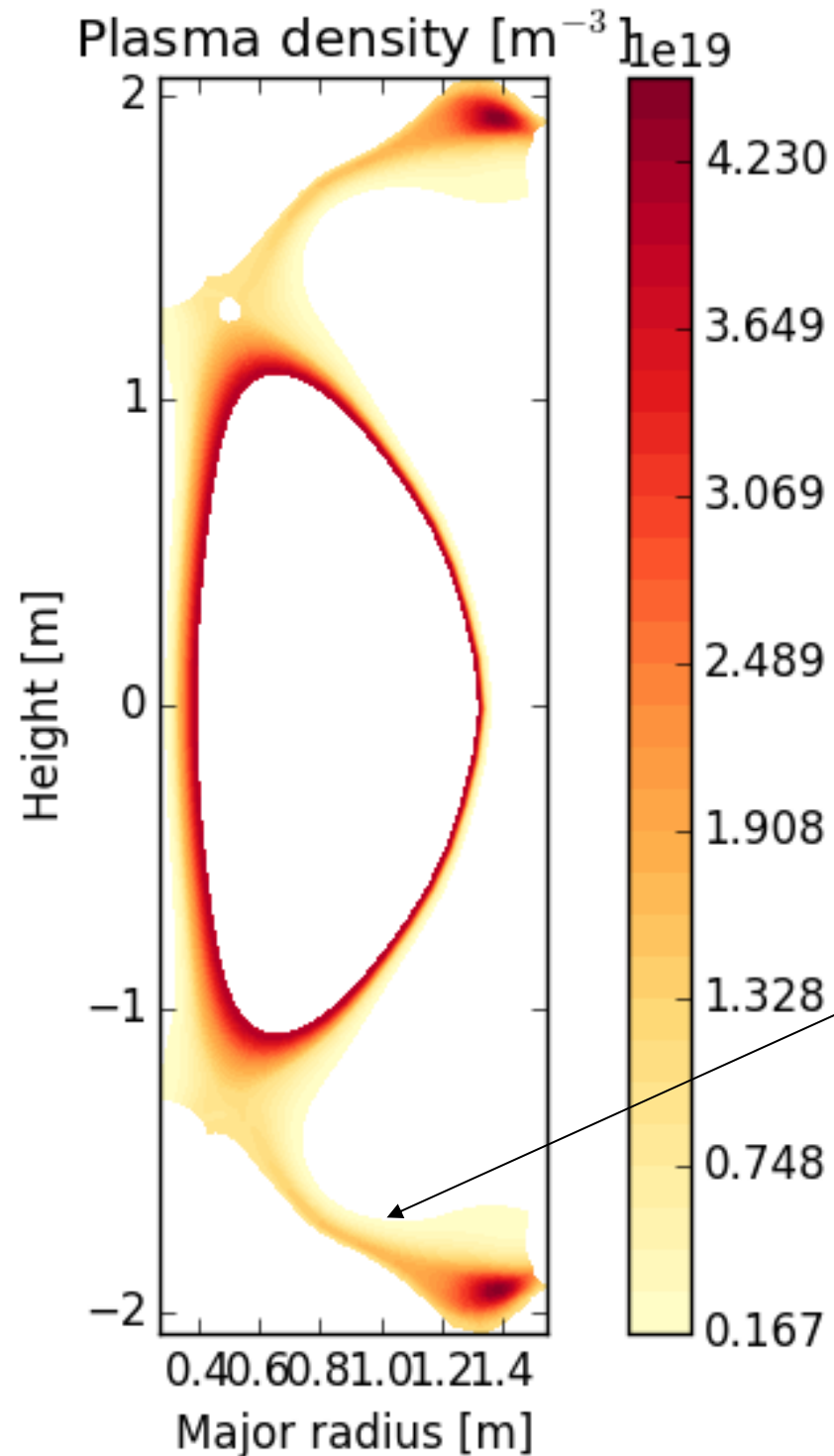


Recycling fraction	80%
Carbon fraction	1%
$n_{e,\text{sep}}$	$1.3 \times 10^{19} \text{ m}^{-3}$
$T_{e,\text{sep}}$	63 eV
D	$0.2 \text{ m}^2/\text{s}$
X	$0.5 \text{ m}^2/\text{s}$

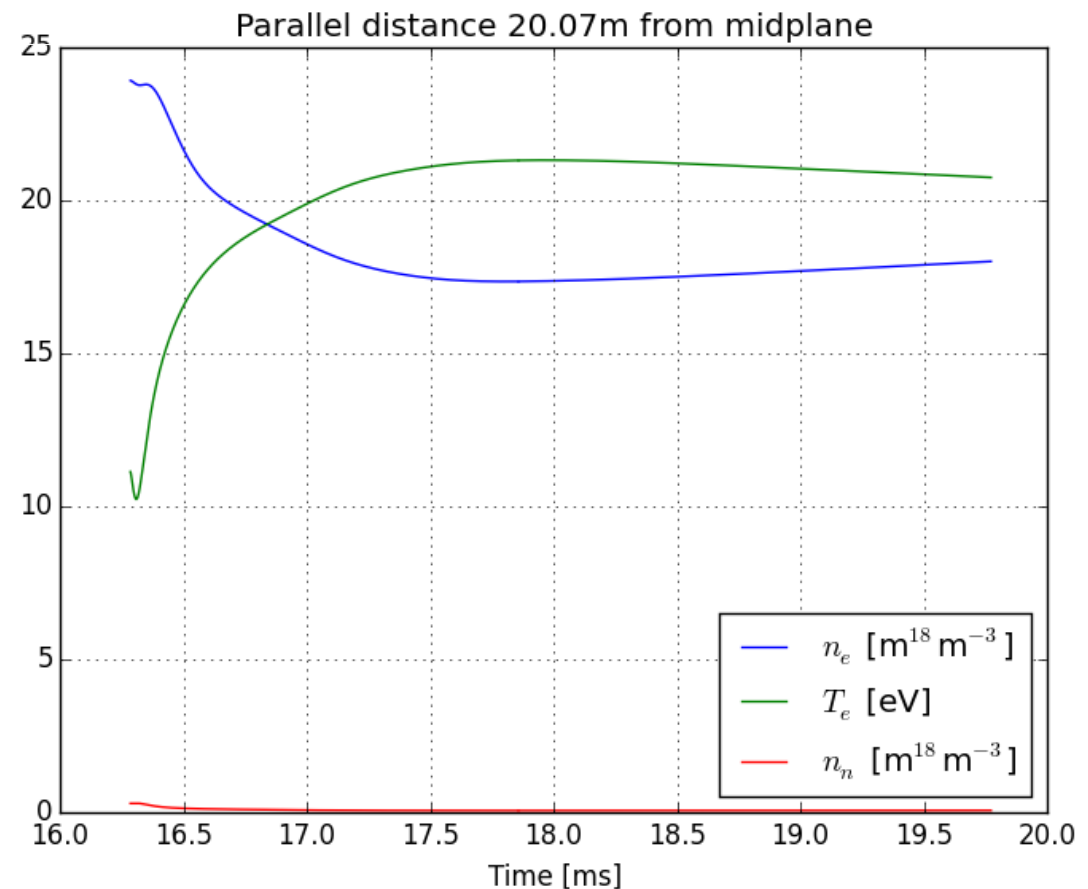


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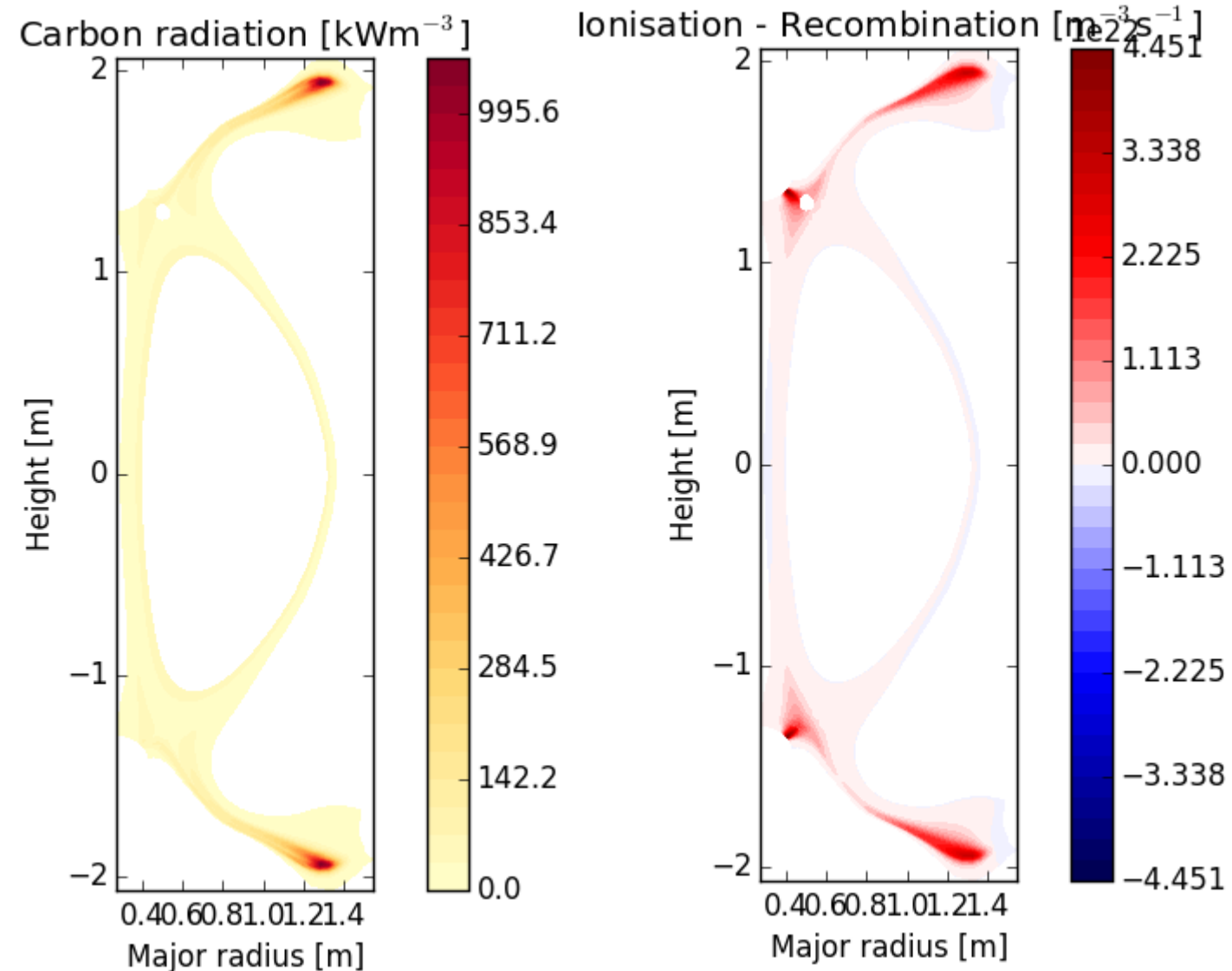
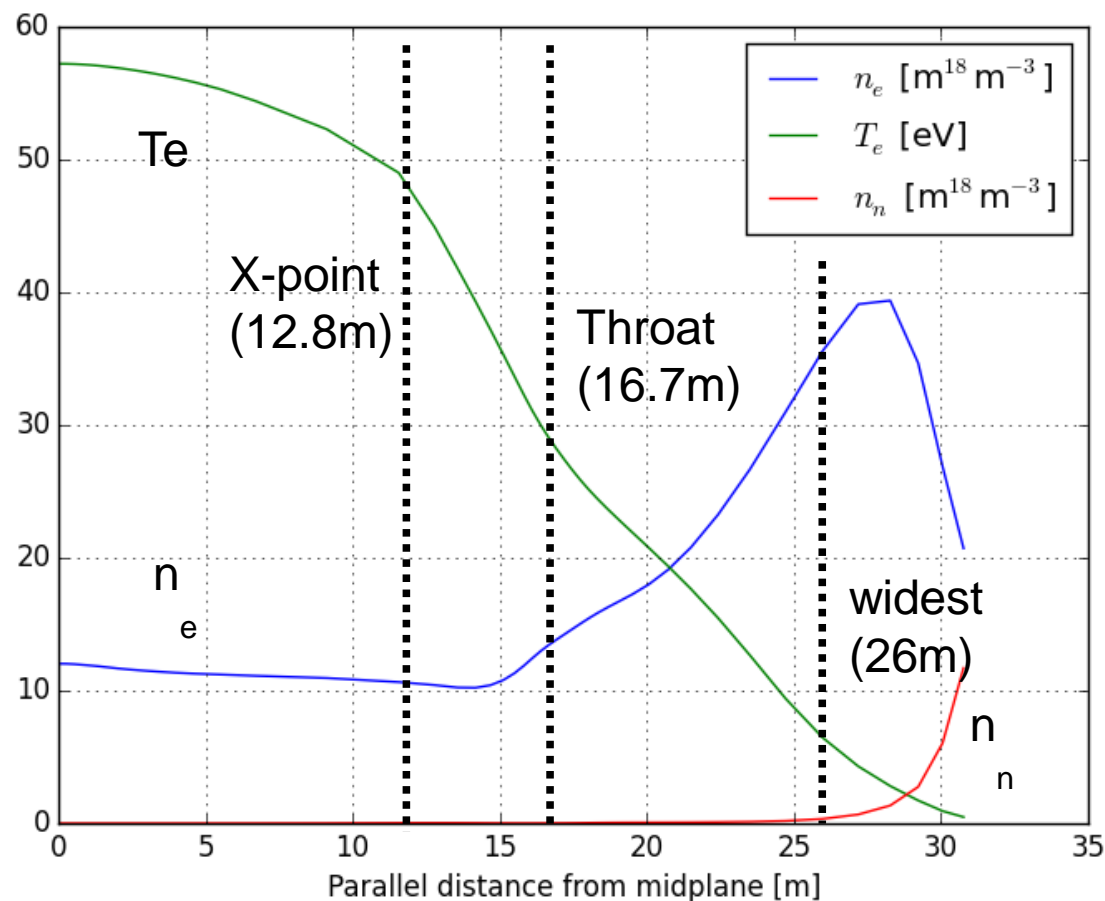
Recycling fraction	80%
Carbon fraction	1%
$n_{e,\text{sep}}$	$1.3 \times 10^{19} \text{ m}^{-3}$
$T_{e,\text{sep}}$	63 eV
D	$0.2 \text{ m}^2/\text{s}$
X	$0.5 \text{ m}^2/\text{s}$



# MAST-Upgrade simulations

- Obtained stable solutions in Super-X geometry
- Net volume recombination near target plates

Input power	497 kW (thermal)
	510 kW (total)
Input particles	$5.7 \times 10^{21}/s$
Carbon radiation	340 kW (67%)
Volumetric loss	56 kW (11 %)



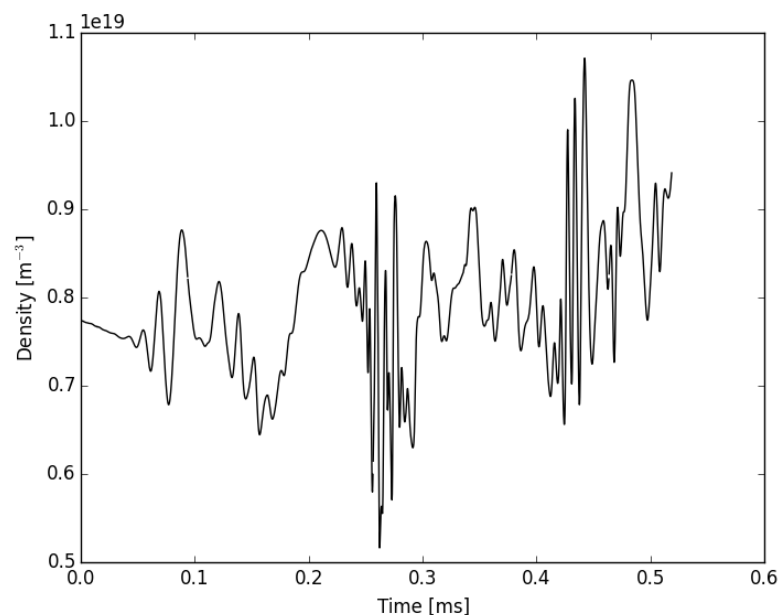
## Future work

- Evolving axisymmetric electric field
- Simulate turbulent transport in Super-X geometry

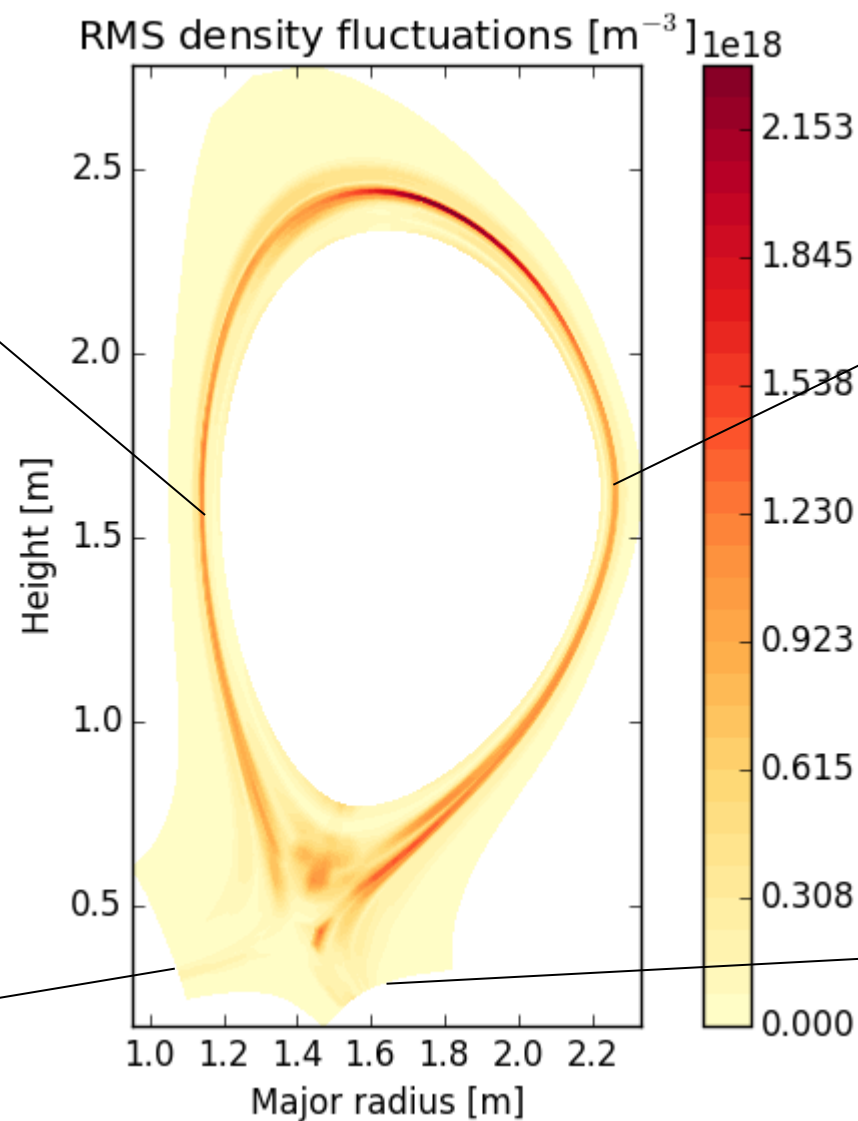
# Turbulence in X-point geometry

Extending the mesh in the toroidal direction, turn off anomalous cross-field transport, and add random noise to vorticity

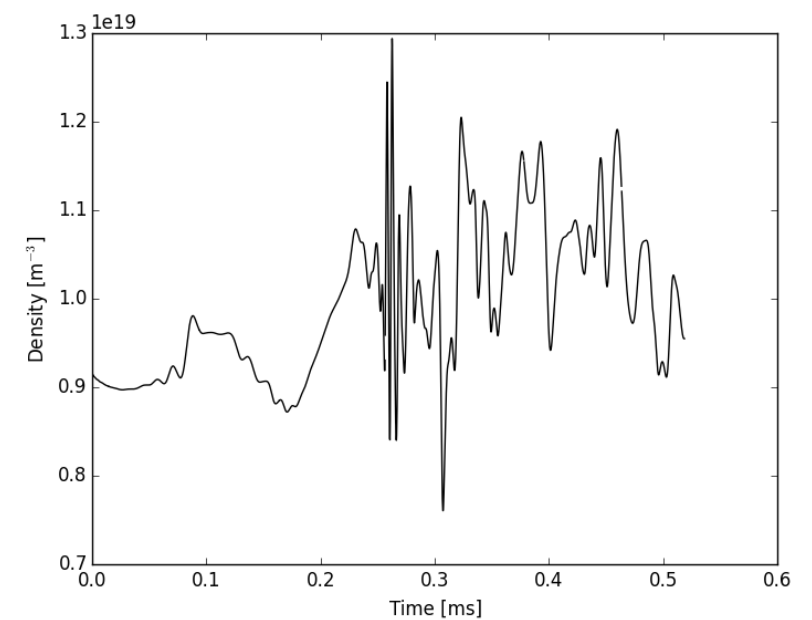
Inboard midplane



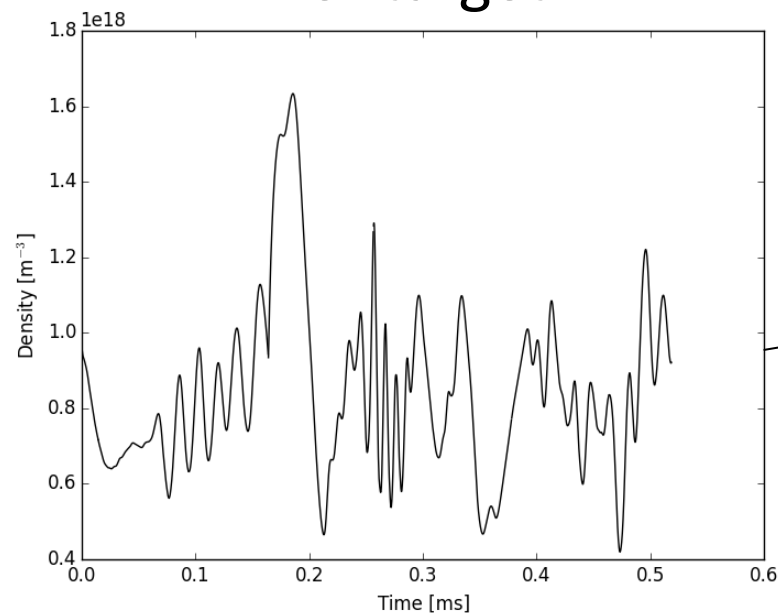
Density at separatrix



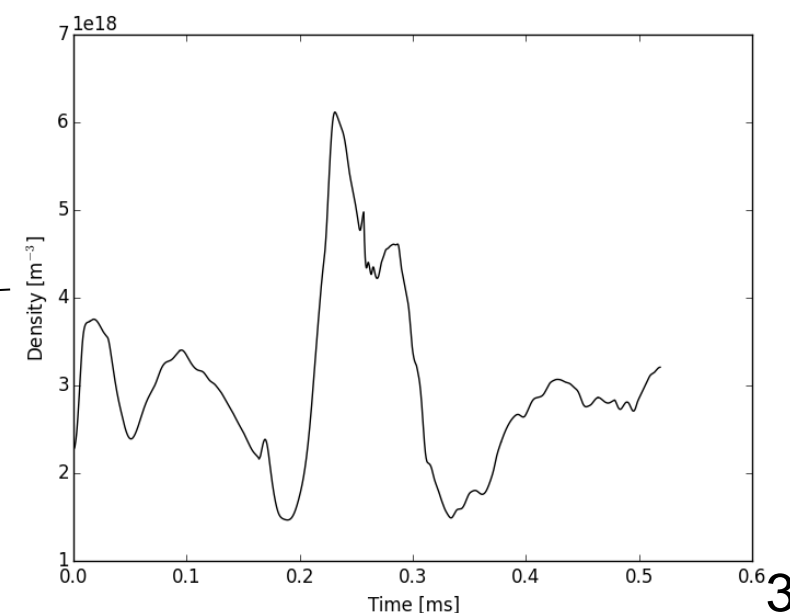
Outboard midplane



Inner target



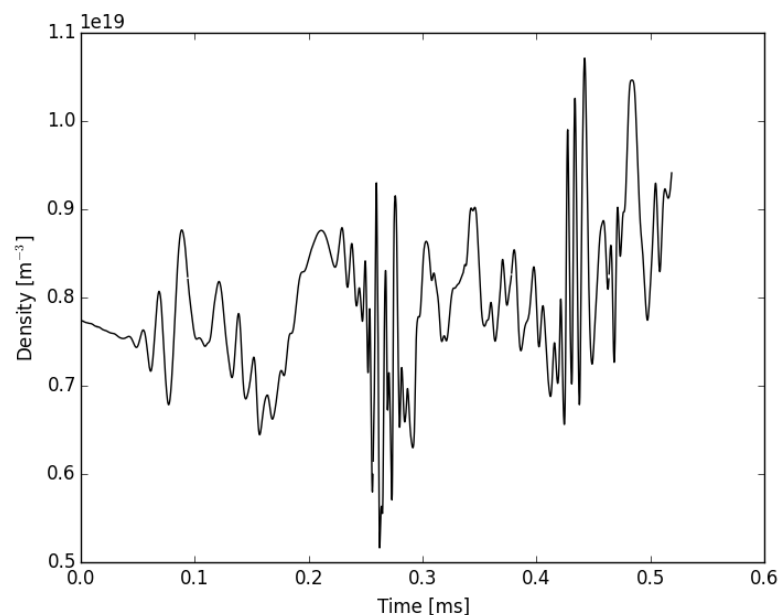
Outer target



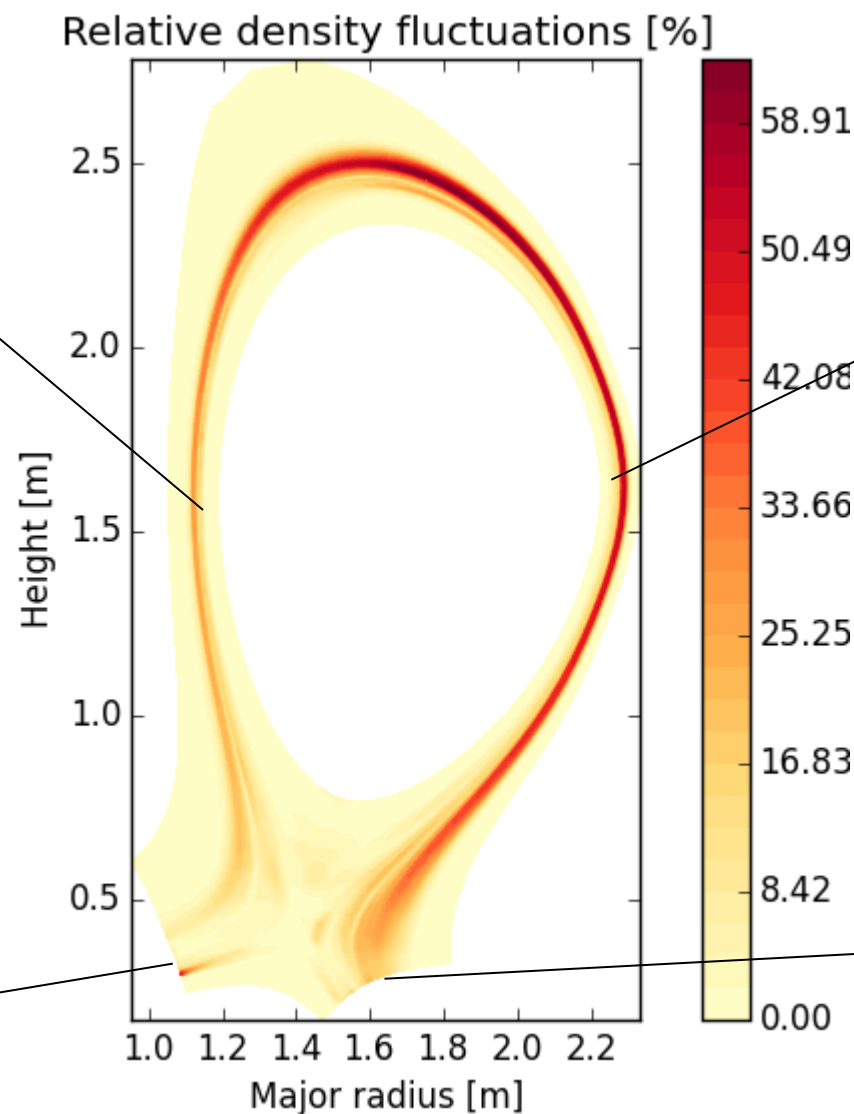
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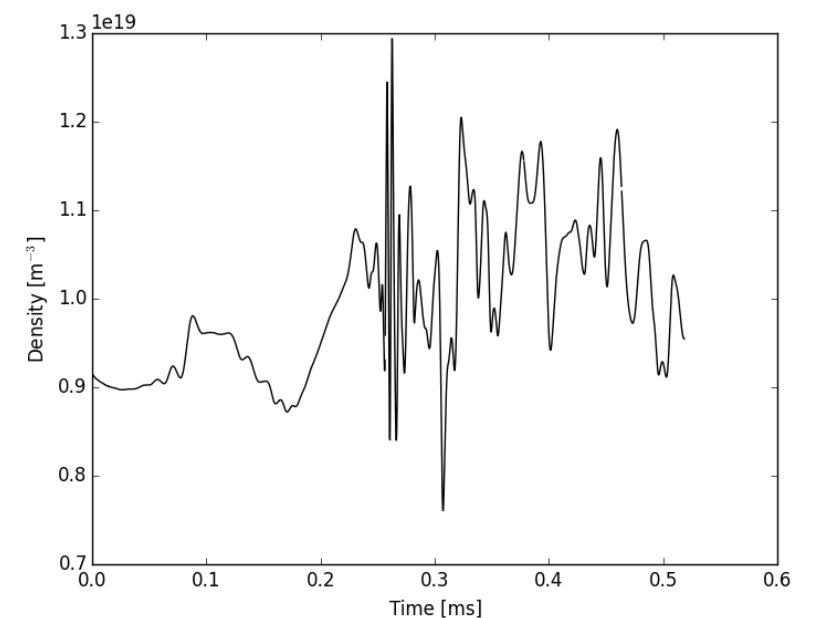
Inboard midplane



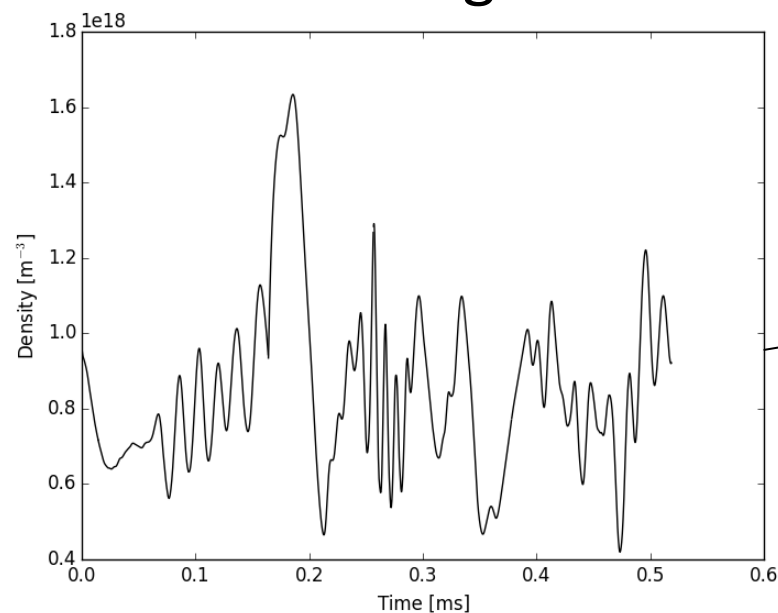
Density at separatrix



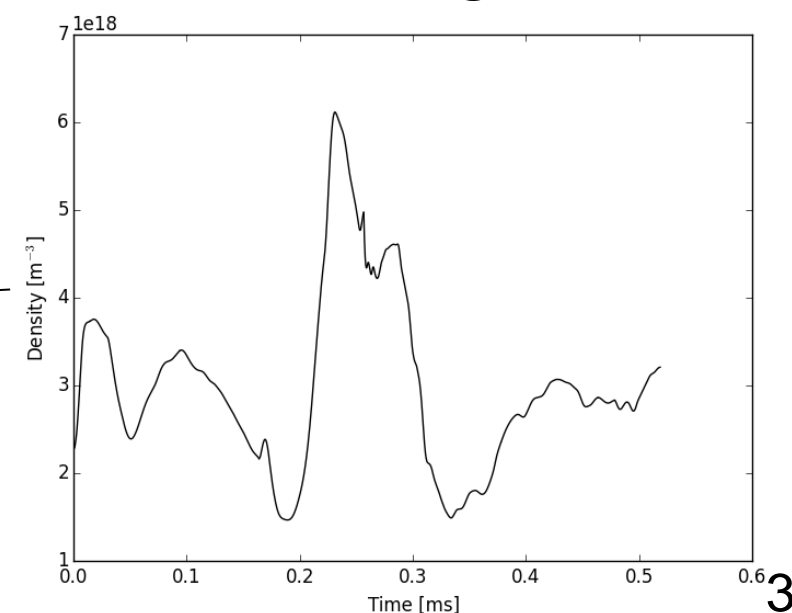
Outboard midplane



Inner target



Outer target

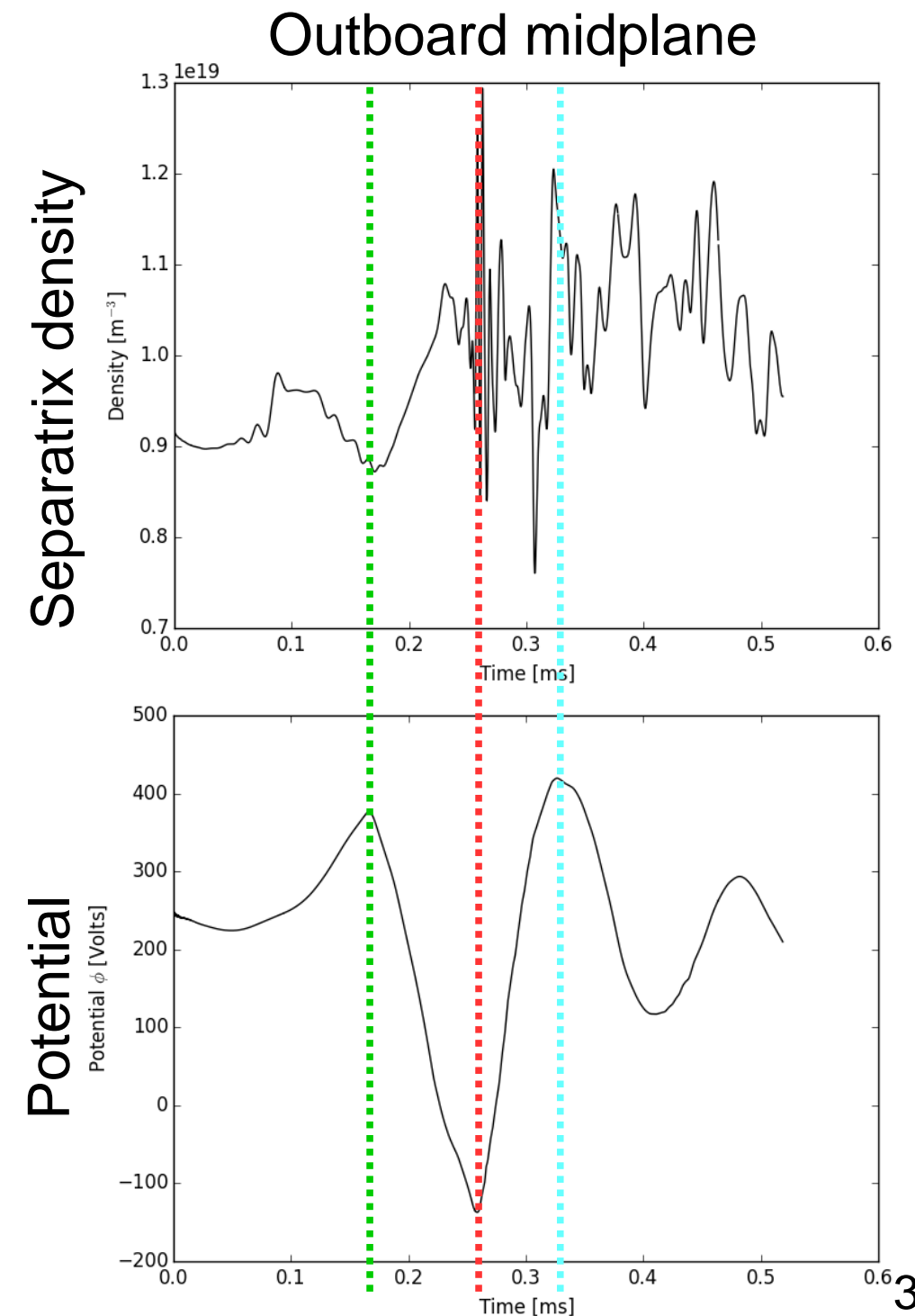
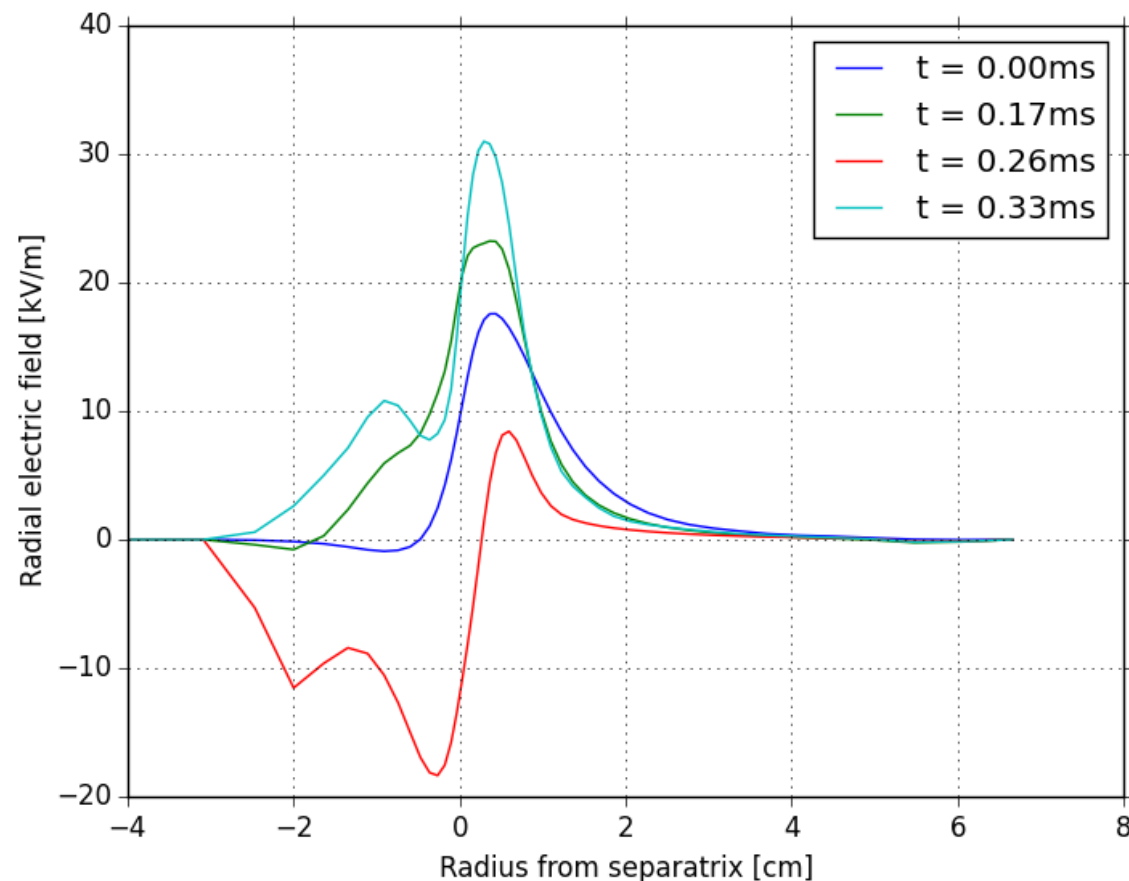




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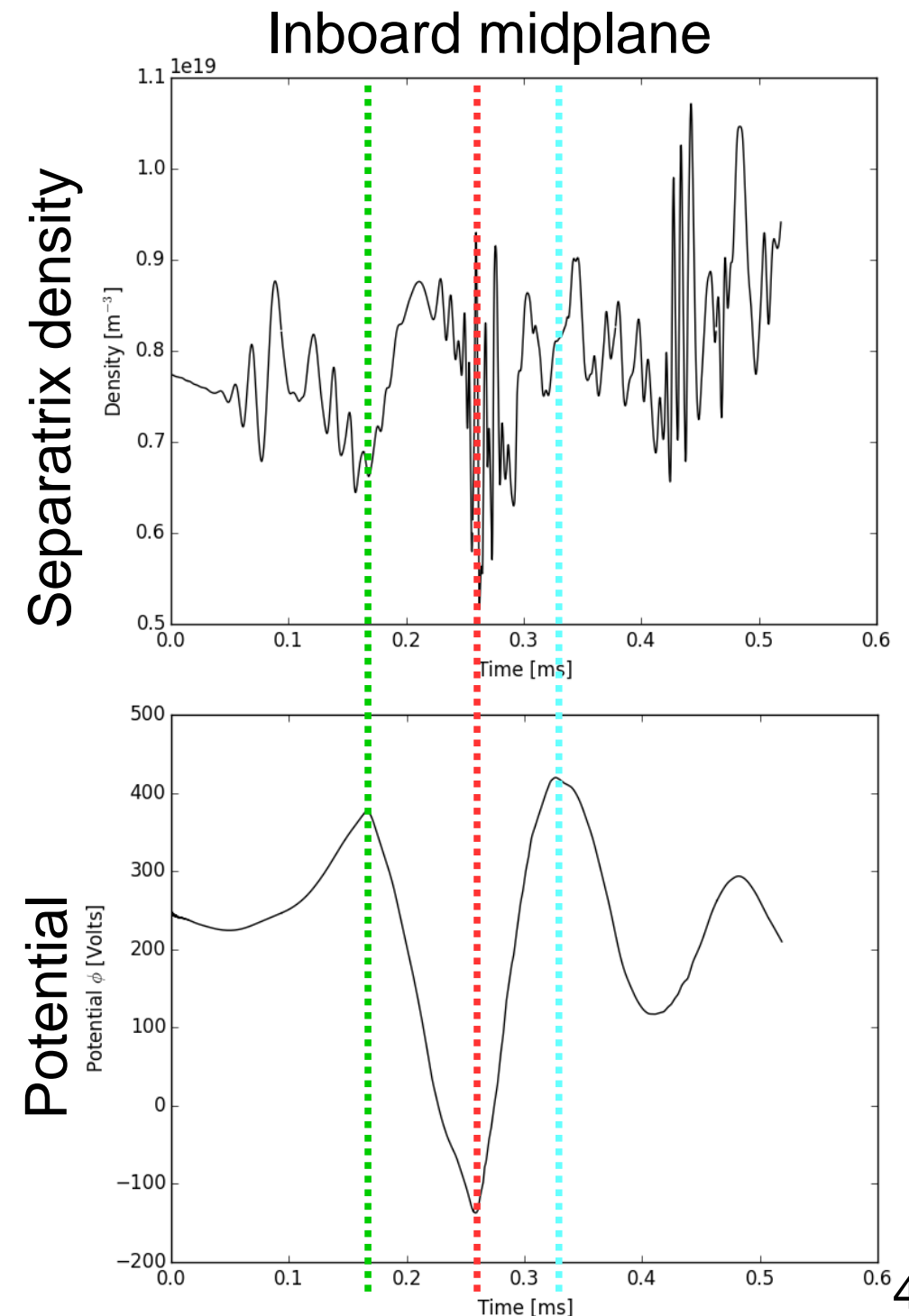
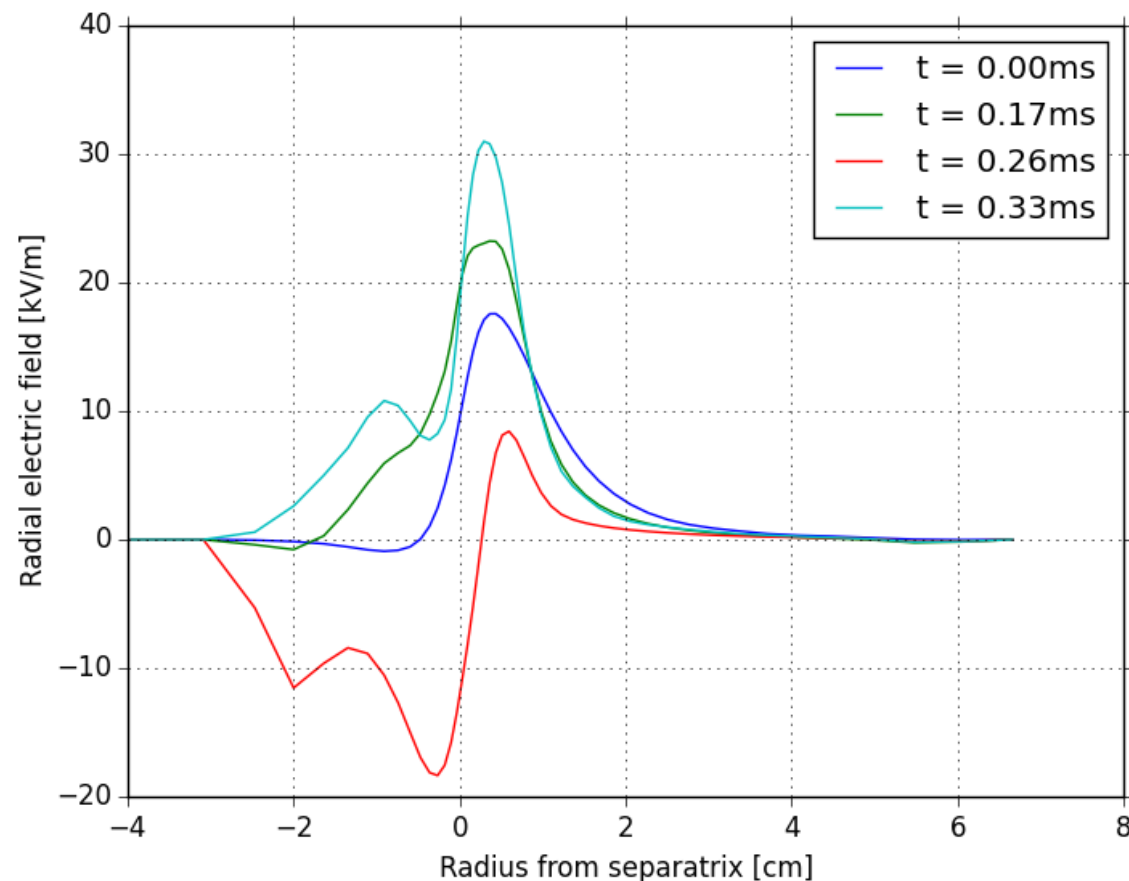
- Fluctuations extended poloidally
- Observed in divertor region, including inner leg PF region
- Large  $n=0$  oscillation in potential



# Turbulence in X-point geometry

Extending the mesh in the toroidal direction, turn off anomalous cross-field transport, and add random noise to vorticity

- Fluctuations extended poloidally
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# Conclusions



- Numerical methods improved for tokamak and non-axisymmetric geometries
- Hermes model being developed (using BOUT++) to study the interaction of transport and turbulence
- Improvements made to model equations and numerical methods allow stable evolution of  $n=0$  electric fields and currents in X-point geometry for the first time in BOUT++
- Fluid neutral model allows study of high recycling regimes. Simulations in linear device demonstrate interaction between plasma turbulence and neutral gas



This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

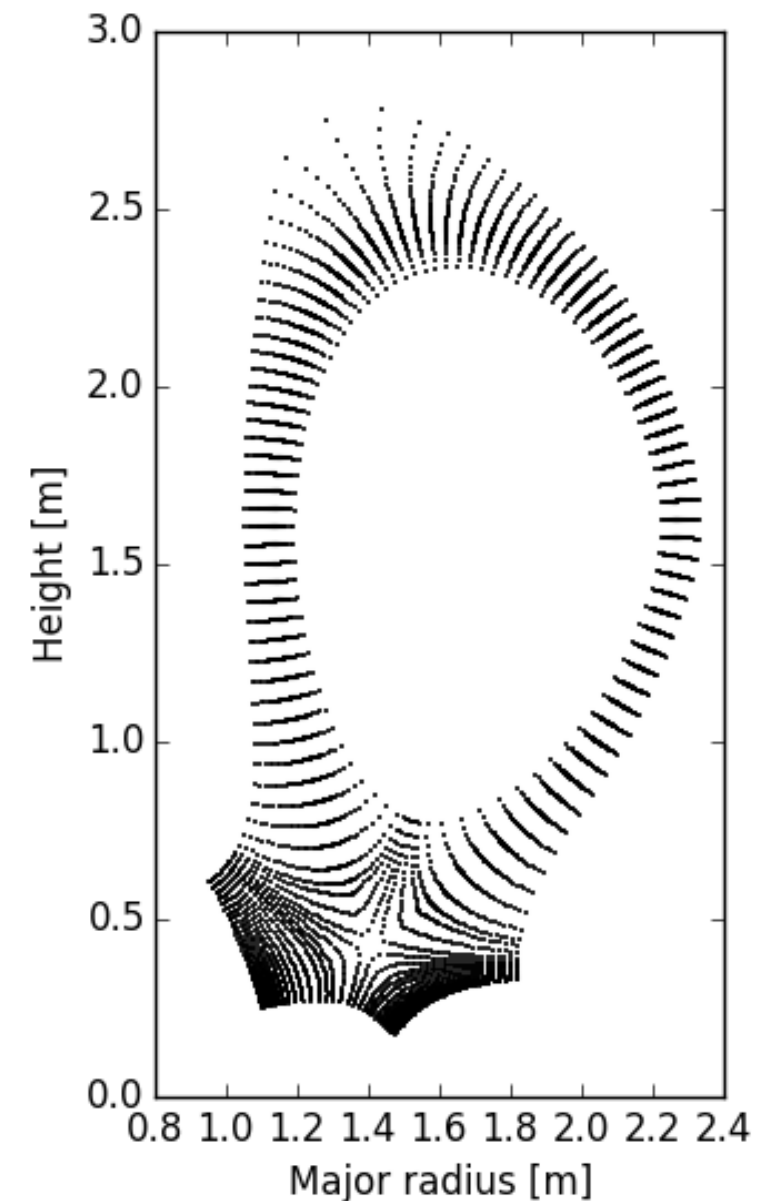
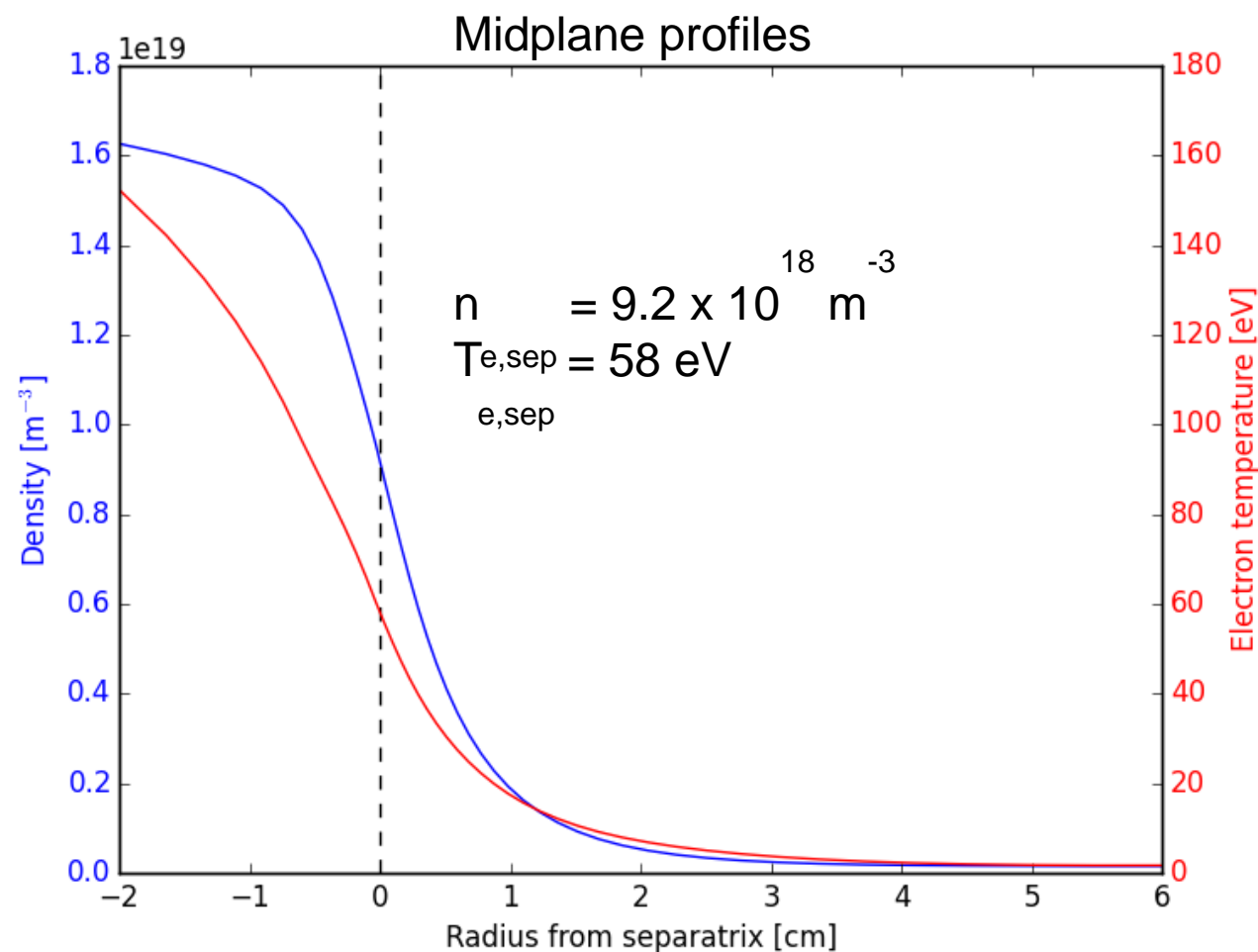


**Extra slides**

# Example equilibrium (DIII-D like)

Hermes can be run as an axisymmetric transport code (e.g. SOLPS, EDGE2D, UEDGE, ...)

- Specify anomalous diffusion coefficients for cross-field transport
- Includes (optional) flux limiters as used in SOLPS
- Start a simulation without electric fields or drifts



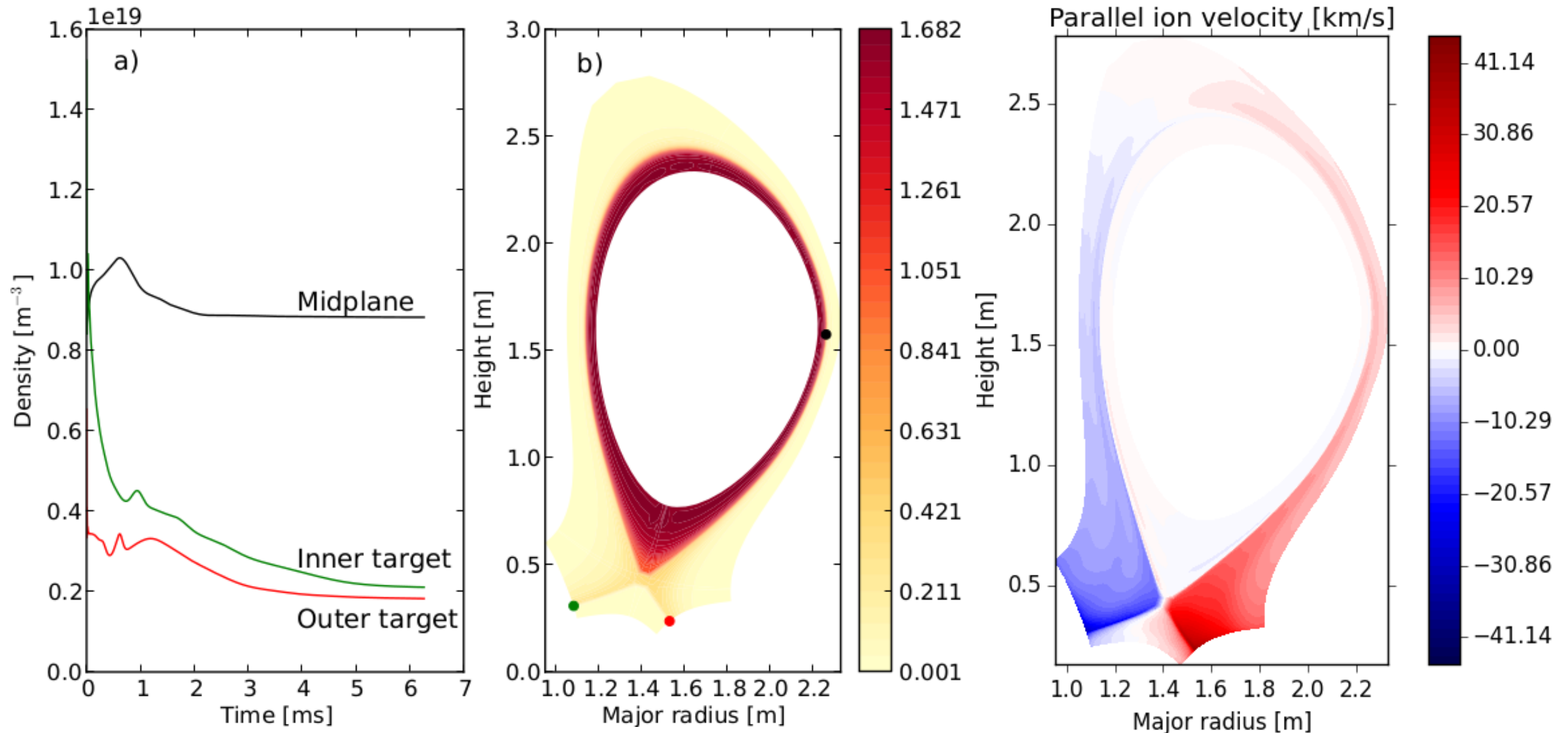
Resolution: 48 x 128 (x 12)



# Evolving axisymmetric profiles

Hermes can be run as an axisymmetric transport code (e.g. SOLPS, EDGE2D, UEDGE, ...)

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# Evolving axisymmetric potential

Initial Alfvénic oscillations  $f \sim 500$  kHz damp on  $\sim 20$   $\mu$ s timescale

Followed by slower oscillation with  $f \sim 6.7$  kHz

Shear Alfvén wave

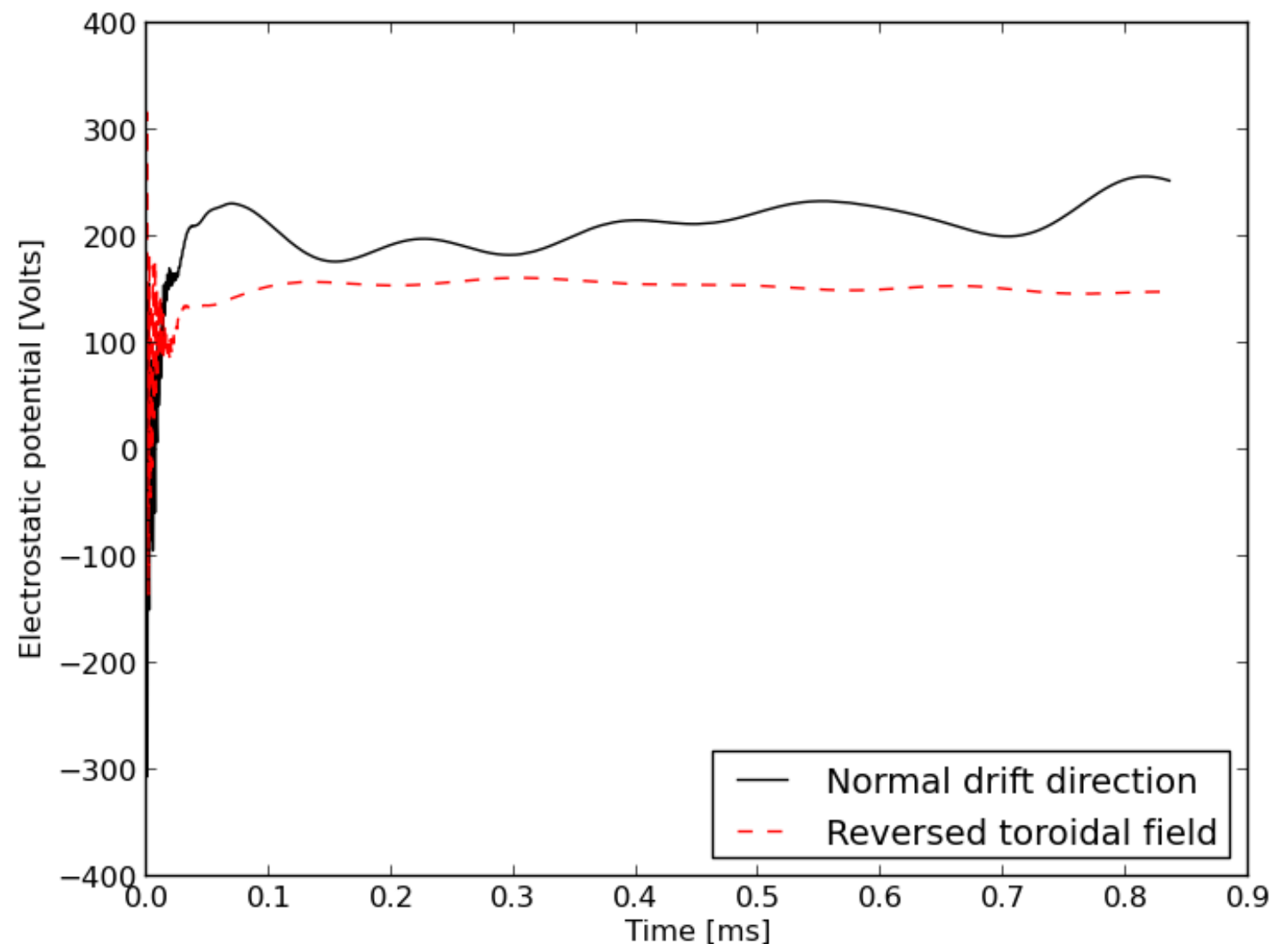
$$f_A = v_A / (2\pi Rq) \\ \simeq 550 - 1100 \text{ kHz}$$

Geodesic Acoustic Mode

$$f_{GAM} = \frac{c_s}{2\pi R} \sqrt{2 + 1/q^2} \\ \simeq 3 - 11 \text{ kHz}$$

Parallel sound wave

$$f_s = c_s / (2\pi Rq) \\ \simeq 0.5 - 2.3 \text{ kHz}$$



# Model includes Alfven waves

Initial Alfvenic oscillations  $f \sim 500$  kHz damp on  $\sim 20 \mu\text{s}$  timescale

Shear Alfven wave

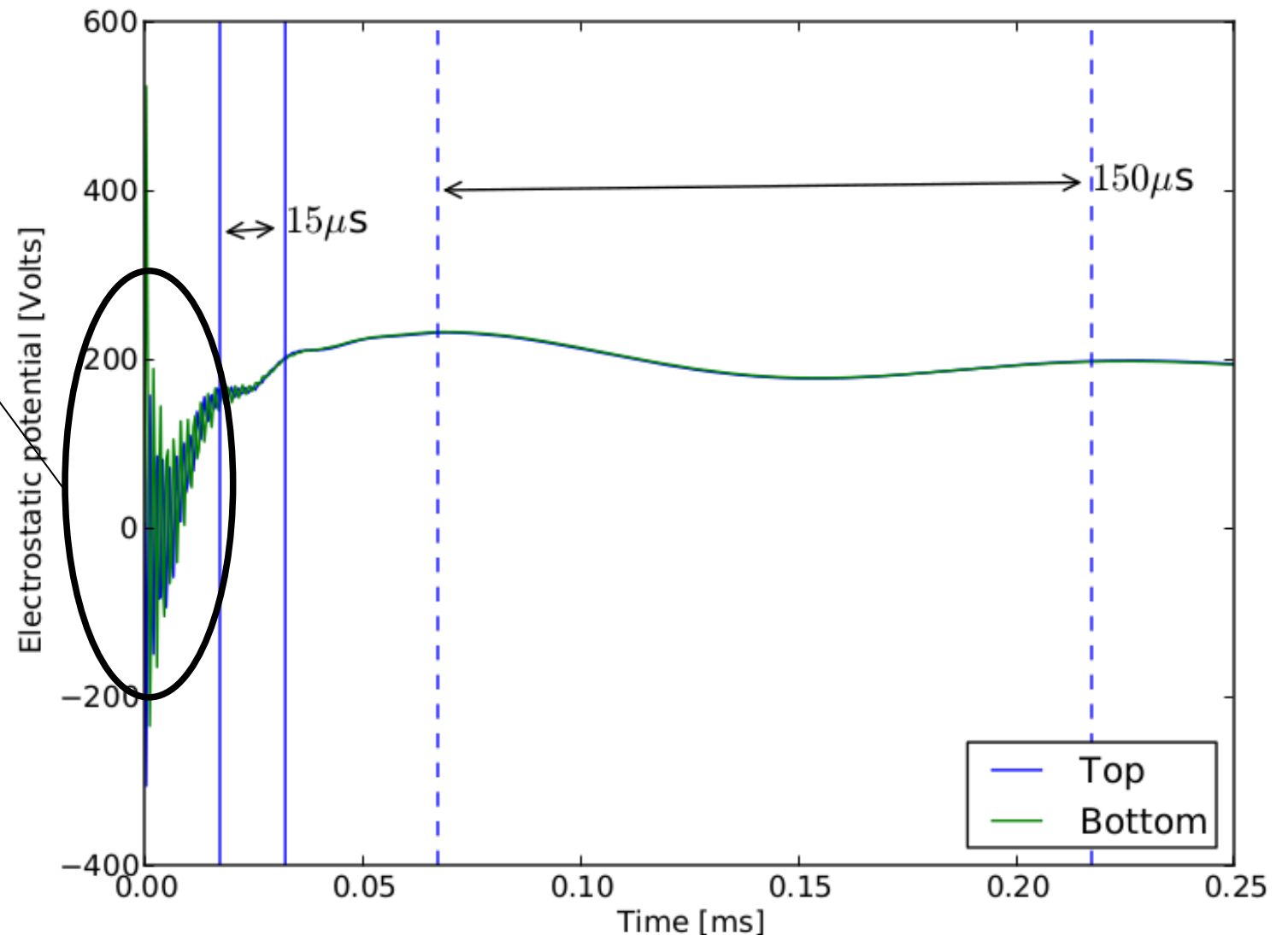
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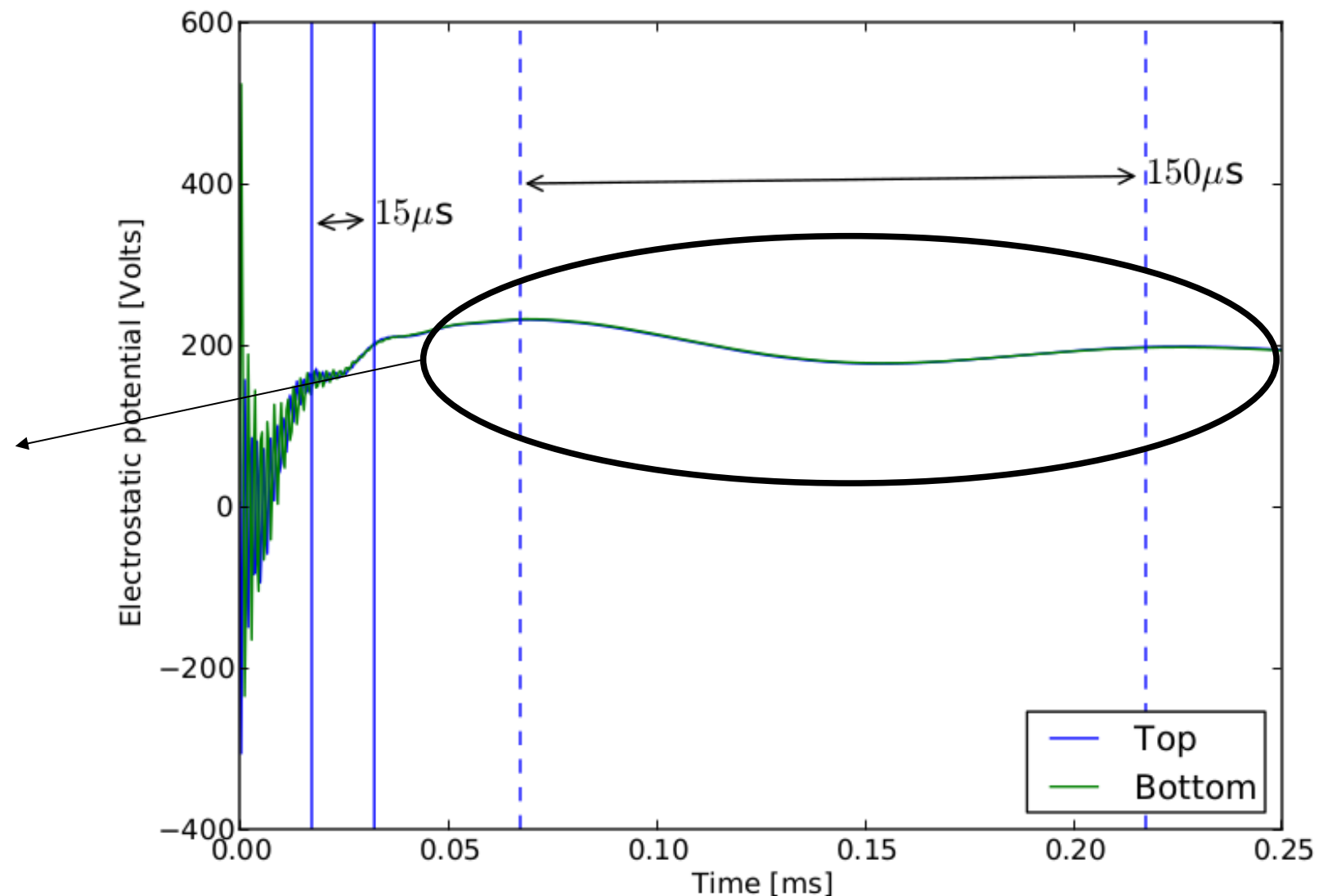
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# Poloidal flows

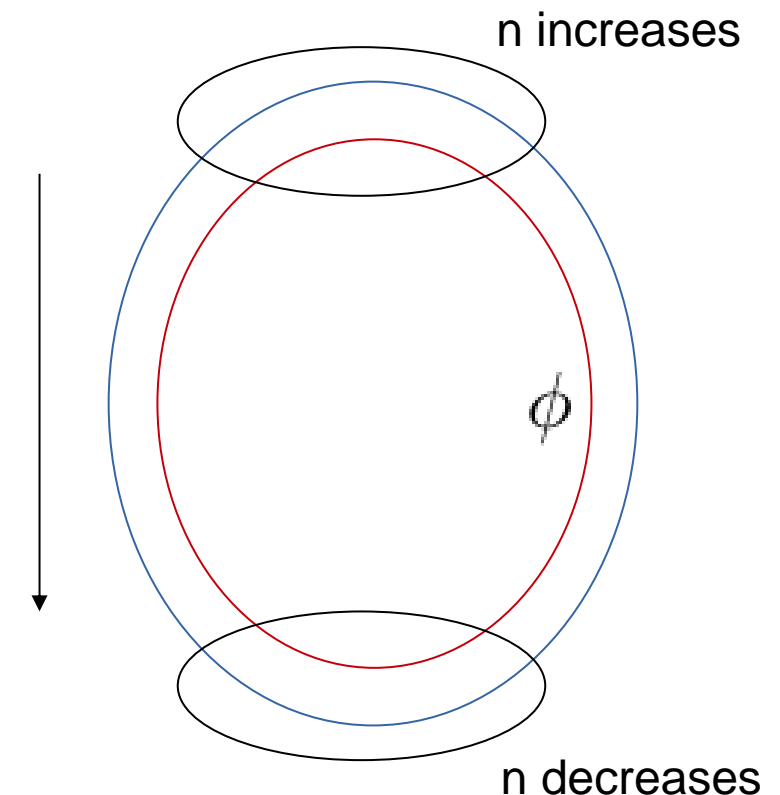
A common way to represent the  $\mathbf{E} \times \mathbf{B}$  flow is

$$\nabla \cdot \left( n \frac{\mathbf{b} \times \nabla \phi}{B} \right) = \frac{\mathbf{b} \times \nabla \phi}{B} \cdot \nabla n + n \left[ \nabla \times \left( \frac{\mathbf{b}}{B} \right) \right] \cdot \nabla \phi$$

Particles added to some cells, removed from others

- In general does not conserve particle number
- Geometry (curvature) need to be restricted

Instead, poloidal flows treated in divergence form  
→ Ensures conservation of particles



Drift-plane motion

$$\begin{aligned} \nabla \cdot \left( n \frac{\mathbf{b} \times \nabla \phi}{B} \right) &= \frac{1}{J} \frac{\partial}{\partial \psi} \left( J n \frac{\partial \phi}{\partial z} \right) - \frac{1}{J} \frac{\partial}{\partial z} \left( J n \frac{\partial \phi}{\partial \psi} \right) \\ &+ \frac{1}{J} \frac{\partial}{\partial \psi} \left( J n \frac{g^{\psi\psi} g^{yz}}{B^2} \frac{\partial \phi}{\partial y} \right) - \frac{1}{J} \frac{\partial}{\partial y} \left( J n \frac{g^{\psi\psi} g^{yz}}{B^2} \frac{\partial \phi}{\partial \psi} \right) \end{aligned}$$

Radial flow due to  
poloidal electric fields

Poloidal flow due to  
radial electric fields

# Tokamaks : Particle conservation

- Conservation of particle number is important in high recycling regimes
- Since total density, pressure is evolved, numerical sources/sinks could affect fidelity of small-scale fluctuations

100% recycling test case

